

POLYNUCLEAR TRANSITION METAL COMPLEXES OF
AMINO- AND IMINOALCOHOLS

A THESIS

Presented to

The Faculty of the Division of Graduate Studies

By

Charles Peter Marabella

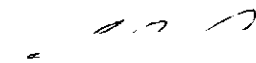
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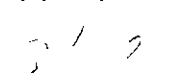
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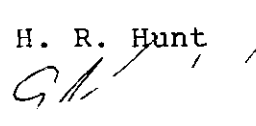
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Summary

Several transition metal complexes with a variety of imino- and aminoalcohols as ligands were investigated. Single crystal X-ray diffraction analyses were carried out on all complexes and variable temperature magnetic susceptibility data were collected for all magnetically interesting compounds.

The two complexes which initiated this study, tetrakis [μ_3 -(7-hydroxy-4-methyl-5-azahept-4-en-2-onato)-copper(II)] butanol (blue unstable crystals) and tetrakis[(methanol) μ_3 -(7hydroxy-4-methyl-5-azahept-4-en-2-onato)nickel(II)] were found to form discrete, tetrameric "cubane" units. The 2-aminoethanol oxygens act as triple-bridging atoms at four tetrahedrally disposed corners of a cube; the metals occupy the remaining four corners. Minor conformational changes in this unit causes the copper complex to exhibit distinctly different magnetic properties.

fac-Tri- μ -(disalicylaldazine)diiron(III) acetone crystallizes as discrete, dinuclear molecules. The crystallographically equivalent iron atoms are octahedrally coordinated. The three binucleating ligands, due to the geometric requirements of each, assume a facial geometry about each metal. The two octahedral coordination spheres do not share a common face but rather are separated by the

distance of the azine bond. Magnetic studies show that the effective moment of the complex exhibits only a slight decrease (5.5-5.1 BM) with temperature (29 - 98°K).

Two metal complexes of 1,3-diamino-2-propanol (DapoH) were structurally and magnetically characterized: trans-[(1,3-diamino-2-propanol)(1,3-diamino-2-propanolato)cobalt(III)] chloride dihydrate and the non-linear copper trimer [bis(N,N'-1,3-diamino-2-propanol)bis(μ -1,3-diamino-2-propanolato) tricopper(II)] iodide methanol. The "monomeric", octahedral cobalt complex forms one-dimensional infinite chains through hydrogen bonding of the trans-oxygens. The complex is diamagnetic. The non-linear trimeric cation contains two monoanionic ligands; each bridges the central copper(II) to a terminal copper(II) through the oxygen (one nitrogen of this ligand chelates to the central copper, the other nitrogen to a terminal copper). The terminal coppers each have their remaining coordination sites filled through chelation of two nitrogens of a neutral ligand; the protonated alcohol group is non-coordinating.

Magnetic studies show that the system is best defined by one coupling constant ($J = -98 \text{ cm}^{-1}$). This indicates that the terminal coppers are not magnetically coupled to any large degree.

A series of four similar complexes were prepared and structurally investigated: (A) $\text{Cu}_2(\text{Dapac})(\text{OAc})$, (B) $\text{Cu}_2(\text{Dapsa})(\text{OAc}):2\text{CH}_3\text{CN}$, (C) $\text{Cu}_2(\text{Dapsa})(\text{OAc}):\text{CH}_3\text{OH}$ and (D) $\text{Cu}_2(\text{Dapsa})(\text{OAc})$ [Note: (Dapac= N,N'-2-hydroxypropylenebis(acetylacetoniminato) and Dapsa= N,N'-2-hydroxypropylenebis(salicylaldiminato)]]. Each dinuclear complex contains two four-coordinate copper(II) atoms bridged by the alkoxide oxygen of the propylene chain and by the oxygens (three atom bridge) of an acetate group. Square planar coordination about each copper(II) is achieved by chelation of the remaining alkoxide oxygens and the imine nitrogens of the binucleating ligand.

Complex A shows the weakest magnetic coupling (probably due to the bent nature of the structure) and complex B, which forms infinite chains, exhibits antiferromagnetic coupling. The structures of C and D exhibit unusual packing and they exhibit antiferromagnetic coupling; their magnetic susceptibilities can be fit to the simple susceptibility equation for a metal dimer.

The final complex reported is $\text{Cu}(\text{DapsaH}):\text{CH}_3\text{CN}$. It forms discrete monomers with the oxygen of the propylene chain protonated and non-coordinating; the remaining four chelating atoms of DapsaH coordinate to the copper(II) in a pseudo-square planar fashion. Steric requirements of the ligand leads to severe twisting as it coordinates and large

deviations from ideal square planar geometry (toward tetrahedral) are observed. The system was assumed to have one unpaired electron with no pathway available for superexchange.

CHAPTER I

INTRODUCTION

History of Complexes

General

The study of "anomalous" magnetic behavior in transition metal complexes was initiated in 1915 by Lifschitz and Rosenbohm (1). They studied copper(II) acetate monohydrate and found it exhibits a subnormal magnetic moment at room temperature (1.43 BM). The structure of the compound was revealed some 38 years later, through X-ray crystallographic studies of van Niekerk and Schoening (2), to be the dimeric compound illustrated in Figure 1. From these studies, the field has now grown to encompass a large area which includes several elaborate structural-magnetic studies of dimers as well as trimers, tetramers and infinite one- and two-dimensional polynuclear complexes (3).

The theory necessary to treat the magnetic properties of these polynuclear systems was complete by 1932. Presently, this theory is being applied to specific isolated compounds and, more importantly, to general structural aspects of series of complexes.

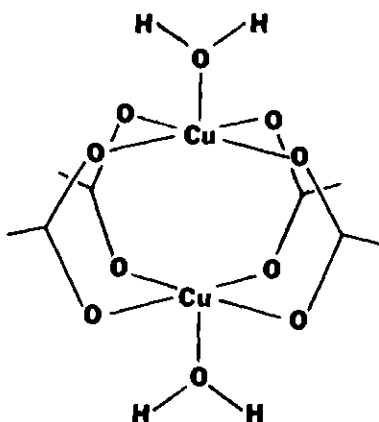


Figure 1. The Dimeric Structure of $[\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}]_2$.

Past studies of polynuclear complexes have repeatedly shown that conclusions based on elemental analysis, spectral and magnetic data alone can lead to incorrect structural assignments. Although structural-magnetic predictive methods can be applied with some success to simple systems, as Hodgson has shown with his series of varied bridging-oxygen angles (4), the need for an exact molecular structure of the molecule is apparent. This is especially true in view of the fact that subnormal magnetic moments of tetramers can be fit to dimeric susceptibility equations by the inclusion of a "paramagnetic impurity" term. It is because of this type of problem that complete single crystal X-ray diffraction analyses should be done if variable temperature magnetic data are to be accurately and confidently interpreted.

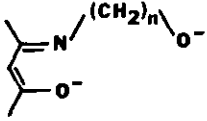
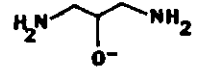
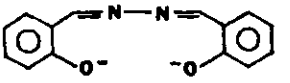
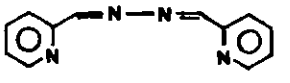
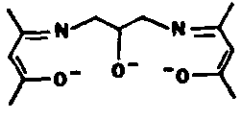
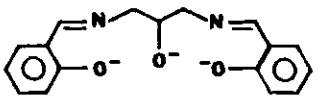
The study of amino- and iminoalcohol transition metal complexes has been a rich area for yielding unusual crystalline polynuclear compounds and different species are often obtained with only minor changes in reaction conditions. Therefore, investigations were undertaken on systems which had been previously prepared but not structurally elucidated. This also led to studies of new complexes which, prior to this report, had not been investigated.

The direct purpose of this investigation is to better understand the correlation between molecular (crystal) structure and magnetic properties of polynuclear transition metal complexes of amino- and iminoalcohols. This is achieved through discriminate synthesis of related crystalline compounds, and the application of single crystal X-ray diffraction and variable temperature magnetic susceptibility methods to these compounds.

A list of abbreviations substituted for ligand names frequently used in this thesis are given in Table 1. The simple abbreviation represents the completely deprotonated anionic form of the ligand and the number of protons present is indicated by the addition of an "H" and a numerical subscript to the abbreviation (i.e. 1,3-diamino-2-propanol = DapoH).

Tridentate O-N-O Donors

Table 1. Abbreviations Used for Ligands.*

Ligand	Abbrev.	Description
	<p>$n=2$; EIA</p> <p>$n=3$; PIA</p>	<p>Dianion of the imine of 2,4-pentanedione and 2-aminoethanol</p> <p>Dianion of the imine of 2,4-pentanedione and 3-aminopropanol</p>
	Dapo	Anion of 1,3-diamino-2-propanol
	DSALZ	Dianion of the diimine of hydrazine and salicylaldehyde
	PAA	Diimine of hydrazine and 2-pyridinaldehyde
	Dapac	Trianion of the diimine of 1,3-diamino-2-propanol and 2,4-pentanedione
	Dapsa	Trianion of the diimine of 1,3-diamino-2-propanol and salicylaldehyde

* "H" added to abbreviation denotes the no. of alcohol groups.

The first study to present magnetic evidence that complexes of tridentate iminoalcohols form polynuclear species was that of Kishita et. al. (5). Although they postulated the 1:1 complex of copper(II) and acetylacetonate-mono(o-hydroxyanil) to be a dimer, it was shown by Barclay and coworkers (6) to adopt the "step" tetramer structure illustrated in Figure 2a. This was the first complex to be structurally characterized which exhibits a subnormal magnetic moment similar to copper(II) acetate monohydrate yet did not have the same type of structure.

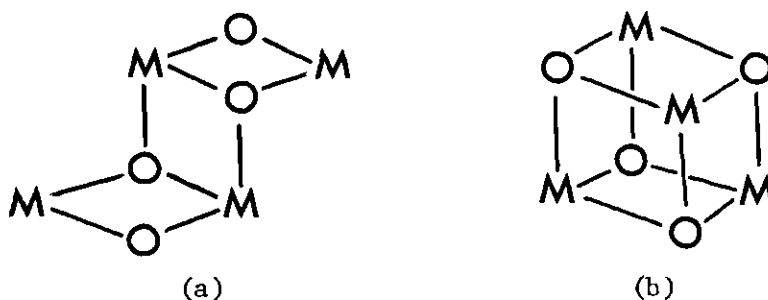


Figure 2. Tetrameric Types of Associations:
(a) Step-like and (b) Cubane-like forms.

In 1966, Jäger prepared several copper and nickel complexes of EIA and PIA (7). Although formally these complexes exhibit coordination numbers of only three, he correctly concluded from spectral, magnetic and molecular

weight determination data that they were polynuclear species. The green, paramagnetic compound $\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})$ was proposed to adopt the polymeric structure shown in Figure 3, whereas green $\text{Cu}(\text{EIA})$ was predicted to have tetrameric associations (no structure proposed).

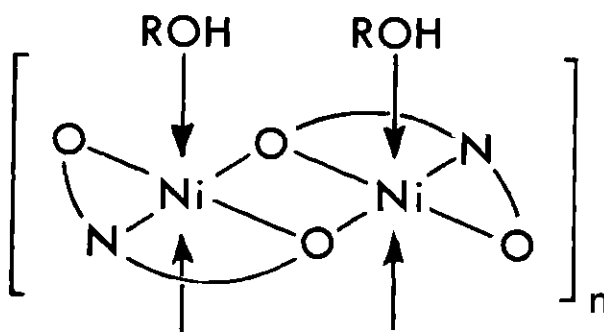


Figure 3. Jäger's Proposed Polymeric Structure of $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_n$.

The first structural studies of these complexes appeared in 1970 (8, 9). The non-solvated, red-brown compounds $\text{Ni}(\text{EIA})$ and $\text{Cu}(\text{PIA})$ are oxygen bridged dimers which are diamagnetic and antiferromagnetically coupled, respectively. The investigations also determined that $\text{Cu}(\text{EIA})$ crystallizes into tetramERICALLY associated cubane-like molecules (Figure 2b). The magnetic and structural comparisons of $\text{Cu}(\text{EIA})$ (tetramer, room temp. moment = 1.87 BM) to $\text{Cu}(\text{PIA})$ (dimer, room temp. moment = 0.41 BM) lead to a better understanding of the importance of the hybridization of the bridging alkoxide oxygen and

its relation to spin exchange via a pi-mechanism. A second, unstable form of Cu(EIA) was also prepared.

Upon the completion of these structural and magnetic studies, several questions arose. What was the nature of the metastable form of Cu(EIA) which had been prepared, but not isolated in the crystalline form? Although Jäger's polymeric structure (Figure 3) of Ni(EIA)(CH₃OH) had been rejected, did the green complex assume a bent dimer with the alcohols occupying the fifth sites of each nickel or did the similarity of properties to those of Ni(acac)(CH₃O)(CH₃OH), which has a cubane structure, indicate a tetrameric form?

In an effort to answer these questions, investigations of these compounds were initialized. Also, the continuing interest of ferromagnetic and antiferromagnetic interactions combined with dimer-tetramer equilibria studies (10) gave other reasons to continue the study of these unusual compounds.

Quadridentate N-N Atom Bridged Species

Several complexes of neutral diimine, two-atom-bridging, quadridentate ligands (Figure 4) have been prepared and structurally characterized. Busch and coworkers initiated the study of this area in 1958 (11). Using PAA and BHA as ligands, they assigned structures based on magnetic and infra-red spectral data.

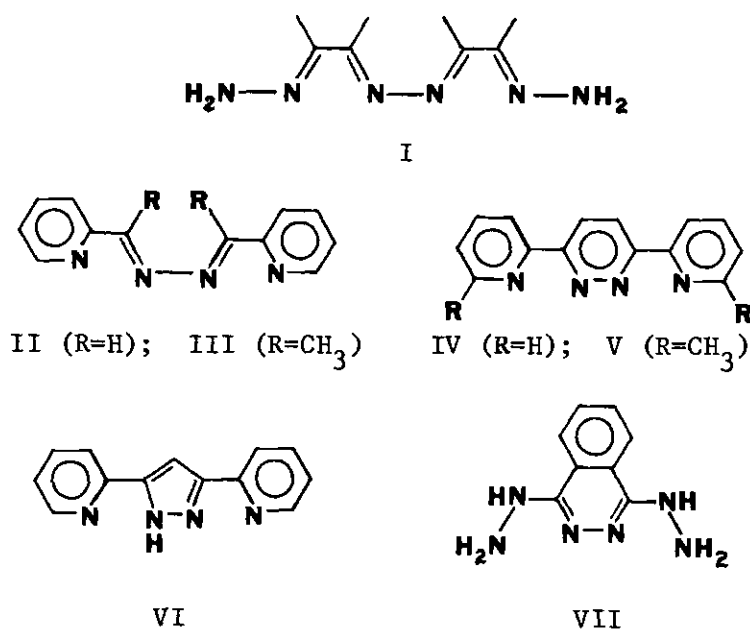


Figure 4. Ligand Structures of BHA (I), PAA (II), PMK (III), dpnp (IV), Me₂dpnp (V), dpplH (VI) and dhph (VII).

They concluded that the complexes crystallize with the following formulas: $M_2(PAA)_3^{4+}$ [$M=Fe(II), Co(II), Ni(II)$], $M(PAA)^{2+}$ [$M=Fe(II), Ni(II), Cu(II)$] and $M_2(BHA)_3^{4+}$ [$M=Fe(II), Ni(II)$]. They assumed the geometries illustrated in Figure 5.

About a decade later Blake et.al. completed the first X-ray structural determination of the cation $[Ni(dhph)]_2$ (12). Armed with this definitive information, they prepared and structurally (via infra-red) and magnetically characterized numerous binuclear nickel(II)

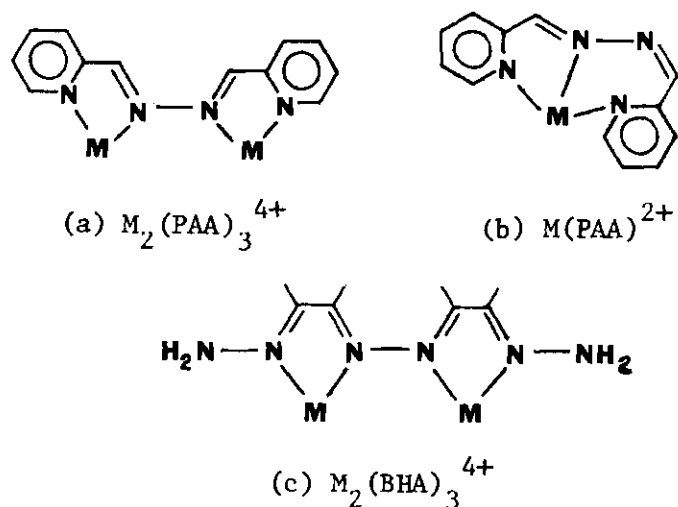


Figure 5. Proposed Coordinations of Neutral Azine Ligands.

(a) $M = Fe(II), Co(II)$ or $Ni(II)$; (b) $M = Fe(II), Ni(II)$ or $Cu(II)$; (c) $M = Fe(II)$ or $Ni(II)$.

complexes of PAA, dppn, Me_2dppn , dpplH and dhph (13). Their concerted efforts lead to the discovery of the first series of $Ni(II)$ binuclear systems to exhibit weak antiferromagnetic coupling ($J/k = -8$ to -34 deg).

Shortly thereafter, cobalt analogs of the binuclear nickel species were studied in depth. Blake and coworkers (14) published magnetic and infra-red results of a few $Co(II)$ complexes of dhph, dppn and Me_2dppn . These, like the $Ni(II)$ complexes, were antiferromagnetically coupled. Concurrently, workers at Cambridge (15) reported an X-ray structure determination of the cation $Co_2(PMK)_3^{4+}$ which had

been synthesized by Stratton four years earlier (16). It has a twisted helical structure, and the twist was attributed to the interactions between the bulky methyl groups (Figure 6).

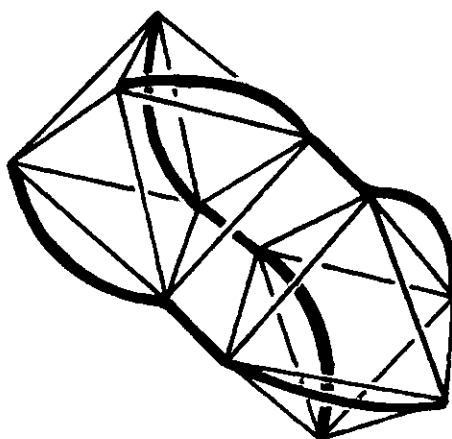


Figure 6. Helical Structure of the Cation $\text{Co}_2(\text{PMK})_3^{4+}$.

No X-ray or other detailed structural reports have appeared in literature for coordination compounds of DSALZ. Some structural suggestions (based on infra-red) made by Sahoo et.al. imply that two distinct structures can be realized, depending upon the identity of the metal (17). They proposed that derivatives of Cu(II), Ni(II) and Co(II) form dinuclear species $[\text{M}(\text{DSALZ})]_2^{4+}$ whereas with Fe(II), a tridentate asymmetric moiety was favored.

Because of the incompleteness of this report and the lack of information on DSALZ and transition metal complexes in general, it was decided to prepare and investigate (structurally and magnetically) these types of compounds.

Dapo Complexes

The majority of investigations of aminoalcohols complexes have been concerned with those of 2-aminoethanol ($\text{EtaH} = \text{NH}_2\text{CH}_2\text{CH}_2\text{OH}$). Few detailed structural and magnetic studies of systems with 1,3-diamino-2-propanol (Dapo) as a ligand have been carried out.

Although Dapo(H) is a simple molecule a variety of coordination modes are possible (Figure 7). As a bidentate ligand, it could chelate to a metal through either the two nitrogen atoms to form a six-membered ring (Figure 7a) or, analogous to EtaH, it could coordinate through one nitrogen and the oxygen (possibly bridging) to form a five-membered ring (Figure 7b,c). The ability of Dapo(H) to function as tridentate ligand is limited, for monomeric species, to fac coordination due to steric considerations (Figure 7d). However, its ability to act as a binucleating moiety has been invoked by at least one research group (18) (Figure 7e).

Another aspect of this ligand is its potential to hydrogen-bond in cases where both a deprotonated and neutral alcohol group are present. This behavior has been

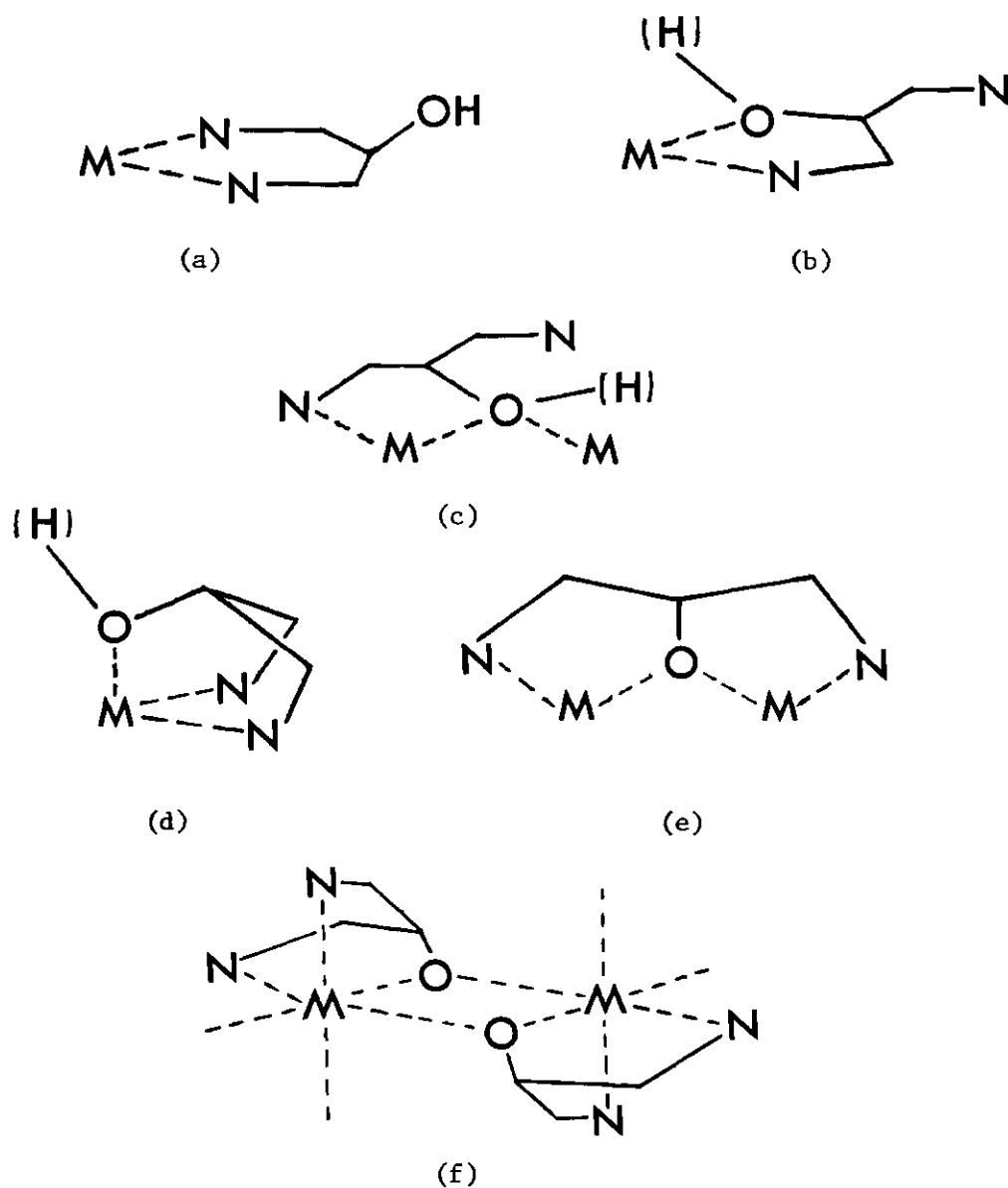


Figure 7. Coordination Modes Possible for Dapo Complexes.

observed for several complexes containing both EtaH and Eta (19). The two types of hydrogen bonded species which have been structurally characterized are sketched in Figure 8.

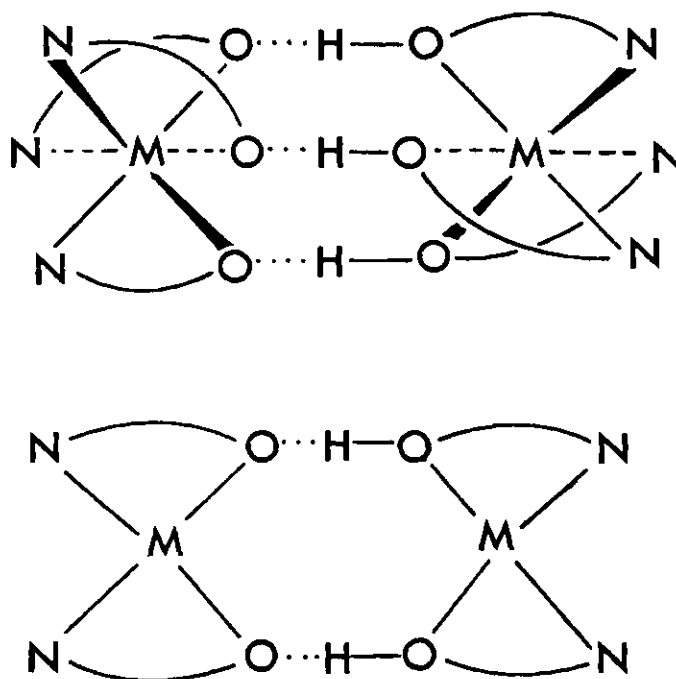


Figure 8. Hydrogen-Bonding in Metal Complexes of Ethanolamine.

The history of metal complexes of Dapo follows a rather long and wandering course, culminating in correct structural characterizations. In 1927, Mann (20) synthesized the compound $[\text{Co}(\text{Dapo})_2]\text{X} \cdot 2\text{H}_2\text{O}$ (where $\text{X} = \text{Cl}^-$, I^- or SCN^- ; originally misformulated as $[\text{Co}(\text{DapoH})_2(\text{OH})_2]\text{X}$

and confirmed by Breckenridge et. al. in 1939 (21)). It was not correctly formulated until 1974 when two groups (22, 23) independently synthesized and characterized the salts shown here:



Both studies concluded, based on spectral and ^{13}C nmr data, that all the complexes in the series adopt a trans geometry.

Näsänen and coworkers reported the preparation of the first structurally characterized copper(II) complex with Dapo as a ligand. The initial paper in 1970 (24) prematurely suggested a dimer (based only on magnetic analysis, density determinations and unit cell parameters). This was followed up by in 1977 (25) by a complete structural determination showing that the complex actually crystallized as a trimer (Figure 9). Treating the complex as an equilateral triangle of copper(II) atoms the complete susceptibility curve could be fitted using the expression:

$$\chi_M = \frac{N\beta^2 g^2}{4 kT} \left[\frac{5 \exp(3J/kT) + 1}{\exp(3J/kT) + 1} \right] + N_\alpha$$

The resulting coupling constant value ($J = -79 \text{ cm}^{-1}$) indicated antiferromagnetic coupling between the copper atoms.

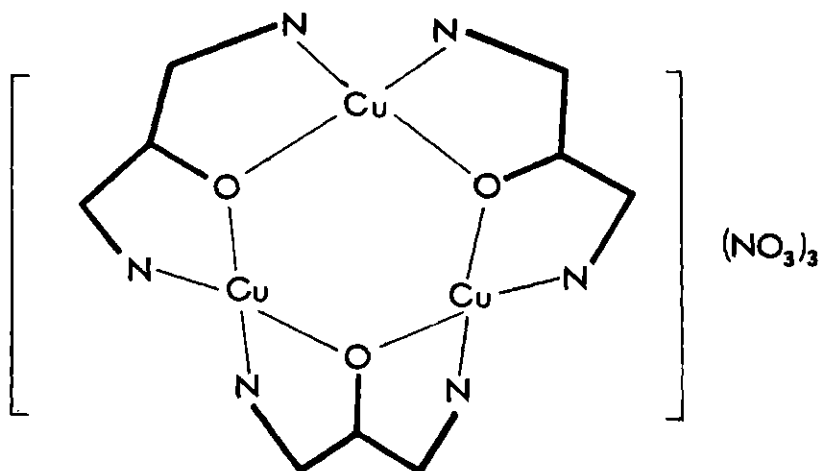


Figure 9. The Cyclic Copper Trimer $[\text{Cu}_3(\text{Dapo})_3](\text{NO}_3)_3$.

The initial impetus for investigating these metal complexes of Dapo was two-fold: to attempt to prepare and study hydrogen bonded polynuclear analogs of the Etah complexes and to shed more light on the little known coordination modes of the Dapo molecule with transition metals.

Charged Schiff Base Diimine Complexes

Most studies of quadridentate, planar ligands have been concerned with the N_2O_2 or N_4 -donor type. This can be ascribed to the recent interest in porphyrin type, bioinorganic metal systems which bind dioxygen. There have been comparatively fewer investigations of charged diimines capable of pentadentate coordination.

Upon recognizing the diverse coordination modes which Dapo(H) assumes in metal complexes, diimine derivatives of this ligand were prepared; 1,3-diamino-2-propanol, condensed with two equivalents of acetylacetone or salicylaldehyde, yielded DapacH₃ and DapsaH₃, respectively.

These ligands could coordinate in two fundamentally different modes (Figure 10):

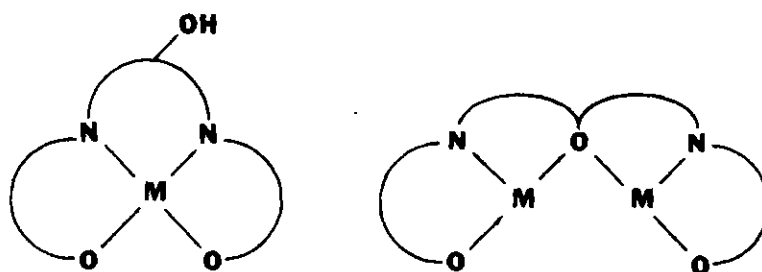


Figure 10. Fundamental Coordination Modes Possible for the Ligands Dapac and Dapsa.

as a tetradentate N₂O₂-donor or as a pentadentate binucleating ligand. The N₂O₂-donor type is illustrated as a monomer but these units could act as building blocks to form dimers, trimers, or tetramers, like the series of complexes studied by both Gruber (26) and Waters (27) (Figure 11).

There is only one report in literature concerning complexes of DapsaH. Dey and Sen (28) assigned, on the basis of infra-red data, a four coordinate structure to a 1:1 complex of palladium and DapsaH.

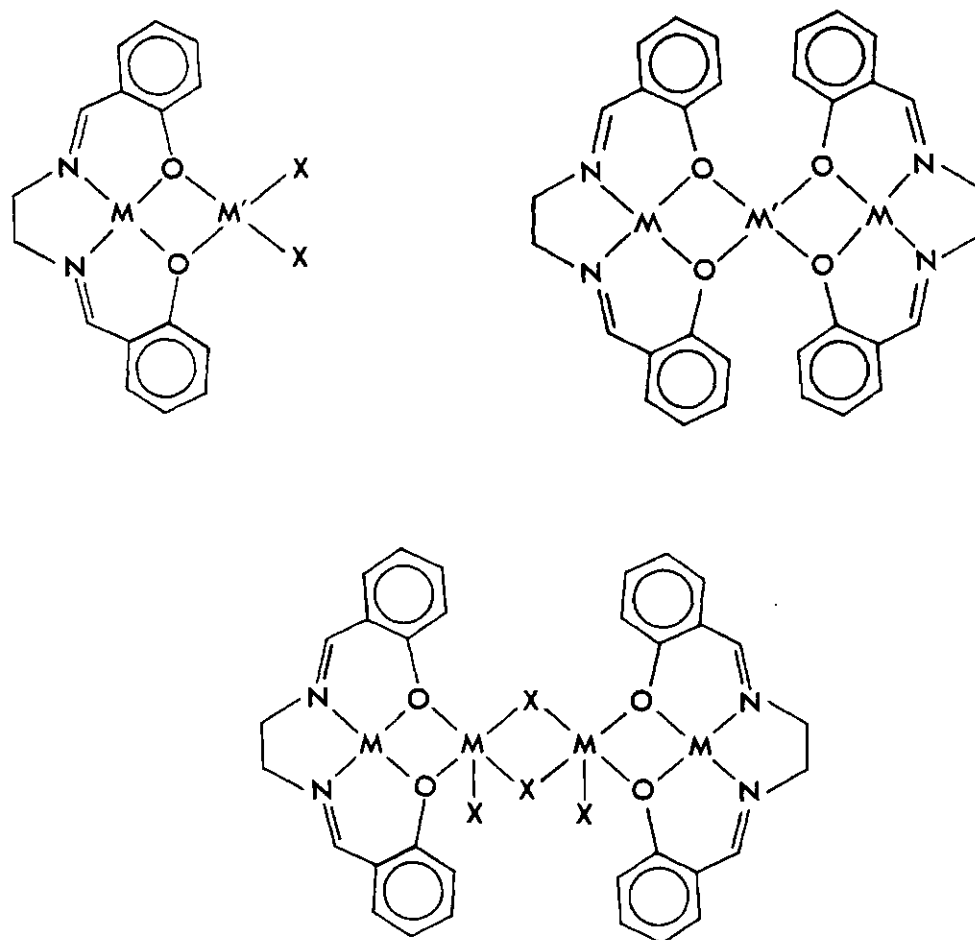


Figure 11. Polynuclear Complexes of salen Which have been Structurally Characterized.

The interesting and unusual transition metal complexes which other Schiff bases form, combined with the paucity of data on such diimine systems, lead to the initiation of a study to elucidate (structurally and magnetically) some copper(II) complexes of Dapac and Dapsa.

The structures of complexes which are described and discussed in this thesis can be conveniently subdivided into four categories.

(1) The tetramERICALLY associated complexes with the imine of ethanolamine and acetylacetone as a ligand: $[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$ and $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_4$.

(2) The two atom bridged complex of iron(II) and disalicylazine: $\text{Fe}_2(\text{DSALZ})_3 \cdot \text{C}_3\text{H}_6\text{O}$.

(3) The mixed ligand complexes containing both the protonated and deprotonated form of DapoH. The ionic compounds: $[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ and $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$.

(4) The complexes of the diimine formed by the condensation of Dapo with acetylacetone or salicylaldehyde: $\text{Cu}_2(\text{Dapac})(\text{OAc})$, $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$, $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$, $\text{Cu}_2(\text{Dapsa})(\text{OAc})$ and $\text{Cu}(\text{DapsaH}) \cdot \text{CH}_3\text{CN}$.

CHAPTER II

EXPERIMENTAL

Elemental Analyses

Carbon, hydrogen and nitrogen analyses were performed by Atlanta Microlab Inc., in Atlanta, Georgia. The results for the metal complexes are summarized in Table 2.

Magnetic Susceptibility Measurements

Magnetic susceptibility data were obtained in vacuum using the Faraday method over a temperature range of 98 to 298 °K. $\text{Hg}[\text{Co}(\text{CNS})_4]$ was used as the calibrant. Diamagnetic corrections applied were those tabulated by Lewis and Figgis (29).

Preparation of Complexes

$[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$

The ligand EIAH_2 was prepared by slowly adding neat 2-aminoethanol to an equimolar amount of neat 2,4-pentanedione. EIAH_2 (5.8 g, 40 mmol) was dissolved with stirring and heating in approximately 100 ml of methanol. This solution was treated with 40 mmol (2.2 g)

Table 2. Results of the Elemental Analyses of Metal Complexes.

Complex	% Found			% Calc.		
	C	H	N	C	H	N
*[Cu(EIA)] ₄	41.14	5.51	6.87	41.06	5.43	6.84
[Cu(EIA)] ₂ ·CH ₃ CN	42.68	5.61	9.29	42.65	5.60	9.33
[Ni(EIA)(CH ₃ OH)] ₄	41.48	6.57	—	41.42	6.53	6.04
Ni(EIA)(C ₂ H ₅ OH)	44.40	6.99	—	43.94	6.98	5.70
Fe ₂ (DSALZ) ₃ ·C ₃ H ₆ O	60.27	4.20	9.23	61.10	4.11	9.50
[Co(Dapo)(DapoH)]Cl ₂ ·2H ₂ O	21.03	6.94	16.21	20.88	6.73	16.24
*[Cu ₃ (Dapo) ₂ (DapoH) ₂]I ₄	13.65	3.73	10.34	13.64	3.63	10.61
Cu ₂ (Dapac)(OAc)	41.26	5.05	6.40	41.18	5.08	6.41
*Cu ₂ (Dapsa)(OAc)	47.39	3.81	5.83	47.39	3.78	5.82
Cu ₂ (Dapsa)(OAc)·CH ₃ OH	46.72	4.35	5.46	46.78	4.35	5.46
Cu ₂ (Dapsa)(OAc)	47.48	3.88	5.94	47.39	3.78	5.82
*Cu(DapsaH)	57.00	4.44	8.01	56.73	4.49	7.79

* These complexes were dried, and formulated as the non-solvated species.

of 85% potassium hydroxide pellets followed by 20 mmol (4.0 g) solid cupric acetate monohydrate. The green microcrystalline material which precipitated was recovered via filtering the hot solution and dried in vacuum. The crude product, 0.2 g, was redissolved in 40 ml of 2-butanol. The blue crystals which formed decomposed rapidly (0.5 to 2h) upon removal from solution. Because of this instability, crystals which were mounted had to be coated with epoxy cement to endure the single crystal X-ray data collection. This crystalline material exhibits a 7-10% weight loss upon decomposition in vacuo.

$\text{Cu(EIA)} \cdot \frac{1}{2}\text{CH}_3\text{CN}$

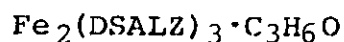
The preparation of this complex is identical to that described in the previous synthesis except the green microcrystalline powder was recrystallized from acetonitrile.

$[\text{Ni(EIA)(CH}_3\text{OH)}]_4$

The method of preparation followed was that of Jager (7). Crystals suitable for single crystal X-ray analysis precipitated from the solution after one day. The unstable crystal mounted, was epoxy coated to avoid crystalline decomposition during data collection.

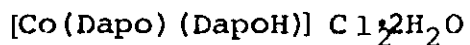
$[\text{Ni(EIA)(C}_2\text{H}_5\text{OH)}]$

The method of preparation of this complex is identical to that previously described except the decomposed material was recrystallized in a mixture of m-xylene and ethanol.



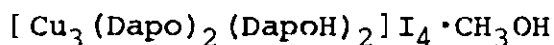
The ligand (DSALZH_2) was prepared by slowly adding hydrazine (85%) to excess (greater than two equivalents) salicylaldehyde in a small amount of ethanol. The exothermic reaction yielded a bright yellow precipitate which was recovered via vacuum filtration and dried in vacuum for several hours. Anal. calculated for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_2$: C, 70.00; H, 5.04; N, 11.66. Found: C, 70.09; H, 5.03; N, 11.54.

To a warmed solution of 1 mmol (0.2 g) iron(II) dichloride tetrahydrate in 35 ml of methanol was added dropwise a solution of 1 mmol (0.25 g) DSALZH_2 in 50 ml methanol. The resulting deep brown solution was filtered hot and allowed to slowly reach room temperature in a Dewar flask. This microcrystalline material was then redissolved in hot acetone and cooled slowly again to yield deep brown crystals suitable for X-ray diffraction studies.

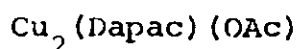


The method of preparation followed was that of Okamoto and Barefield (23). To induce needle-like crystals

of good quality, the final solution was slowly evaporated in air rather than with a stream of nitrogen.



Cupric acetate monohydrate, 5 mmol (1.0 g), and 15 mmol (1.4 g) of 1,3-diamino-2-propanol were combined in approximately 75 ml of methanol. Subsequent addition of an aqueous solution of 15 mmol (2.2 g) of KI to the deep blue solution, followed by slow evaporation in air, yielded crystalline material adequate for single crystal X-ray studies.



The ligand Dapach₃ was prepared by treating 40 mmol (4.0 g) of 2,4-pentanedione in 50 ml of ethanol with 20 mmol (1.8 g) of 1,3-diamino-2-propanol. The volume of the solution was reduced with a rotary evaporator and the ensuing microcrystalline powder was washed with cold acetone. Anal. calculated for $\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}_3$: C, 61.38; H, 8.74; N, 11.02. Found: C, 61.39; H, 8.72; N, 11.01.

A hot solution of 50 ml of ethanol and 5 mmol (1.0 g) of cupric acetate monohydrate was treated with 6 mmol (1.5 g) Dapach₃ in 25 ml of ethanol. The resulting deep blue solution was filtered hot and slowly brought to room temperature in a Dewar flask. After several hours, the solution produced blue, uniform crystals suitable for single crystal X-ray studies.

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$

The ligand was prepared by slowly adding 5 ml of an ethanolic solution of 10 mmol (0.9 g) DapoH to 40 ml of a hot ethanolic solution containing 20 mmol (2.5 g) of salicylaldehyde. (This preparation was followed in all subsequent syntheses in which Dapsa-metal complexes were prepared.) This deep yellow solution was then added dropwise to 13 mmol (2.6 g) of cupric acetate monohydrate dissolved in approximately 75 ml of ethanol. A small portion of the green powder which separated from the dark green solution was immediately dissolved in 10 ml of acetonitrile and evaporated to dryness. The resulting dark green crystals decomposed after being exposed to the air for a few days. Therefore, the crystal mounted for X-ray studies was coated with epoxy cement.

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$

To 50 ml of a hot methanolic solution of 10 mmol (2.0 g) of cupric acetate monohydrate was slowly added a solution containing 5 ml of a methanolic solution (5 mmol, 1.5 g) of DapsaH₃ (Prepared as described above but using methanol as the solvent.) The ensuing dark green solution was filtered hot and left open to the air. Within a few hours, dark green uniform crystals separated from solution.

$\text{Cu}_2(\text{Dapsa})(\text{OAc})$

The non-solvated form in this series of compounds was prepared as follows: To a hot suspension of 10 mmol (2.0 g) of cupric acetate monohydrate and 50 ml of acetonitrile was added 10 ml of an ethanolic solution containing 5 mmol (1.5 g) DapsaH₃. The dark green solution which immediately ensued was filtered hot and brought to room temperature overnight in an insulated Dewar flask. The next day crystals suitable for single crystal X-ray diffraction studies were evident.

Cu(DapsaH) · CH₃CN

This monomer was prepared by treating 150 ml of a hot ethanolic solution of 25 mmol (5.0 g) of cupric acetate monohydrate with 20 mmol (6.0 g) of an ethanolic solution of DapsaH₃. The olive green powder which suddenly precipitated was recovered and a small amount of it was dissolved in hot acetonitrile. Crystals suitable for single crystal X-ray diffraction studies were obtained upon allowing the acetonitrile solution to slowly reach room temperature in a Dewar flask. The crystalline material decomposed very quickly (10 - 60 min) once removed from the solution, so the crystal was coated several times with epoxy cement to prevent decomposition.

Crystallographic Information

General

The intensity data for all structures were collected on a Syntex P2₁ four circle diffractometer equipped with a highly ordered graphite monochromator (Bragg 2θ angle = 12.2 degrees) using MoK α radiation (λ = 0.71069 Å) at a takeoff angle of 6.5 degrees. The unit cell parameters and orientation matrix were determined on the accompanying Nova 1200 Series computer (8K memory).

Unless otherwise specified, fifteen reflections, located from initial phi rotation photographs and machine centered, were used in the least squares refinement of the lattice parameters and the orientation matrix. Once the crystal system was determined, several zero level axial reflections were collected and omega scans were completed to assure that the crystal had a satisfactory mosaic spread (i.e. peak widths at half height of less than 0.35 degrees). Three axial reflections were then chosen as standards to be monitored (set to recenter if intensity falls below 92% of the original value) after every 97 reflections. The scan width was set at 2.0 degrees for all structures and this was sufficient to collect all of the peak intensity.

Intensities were calculated from the total scan count (CT) and from initial (bdg 1) and final (bdg 2) background counts by the relationship:

$$I = CT - (bdg1 + bdg2)$$

The intensities were assigned standard deviations according to the equation:

$$\sigma(I) = [CT + (bdg1 + bdg2)]^{1/2}$$

Important crystallographic data for each structure determined are presented in Table 3.

Standard programs (30) were executed on the CDC Cyber 74 System. The necessary scattering factors for all atoms except hydrogens (31) were taken from those tabulated by Cromer and Waber (32). The scattering factors for all atoms in the structures with a larger atomic number than oxygen were corrected for the real and imaginary anomalous dispersion components (33).

Agreement factors were defined in the usual way as:

$$R = (\sum ||F_o| - |F_c||) / (\sum |F_o|)$$

and

$$R_w = [\sum w(|F_o| - |F_c|)^2 / \sum w(|F_o|)^2]^{1/2}$$

where $w = 4I / \sigma(I)^2$. In all least squares refinements, the quantity minimized was $w(|F_o - F_c|)^2$.

Table 3. Important Crystallographic Information for the Structures Solved and Refined for this Thesis.

	$[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$	$[\text{Ni}(\text{EIA})\text{CH}_3\text{OH}]_4$	$\text{Fe}_2(\text{DSALZ})_3 \cdot \text{C}_3\text{H}_6\text{O}$	$[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$	$[\text{Cu}_3(\text{Dapo})(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$
COLOR	blue	green	dk. brown	red	blue
APPROX. SIZE (mm)	.75 x .50 x .50	.50 x .40 x .30	.50 x .50 x .30	.50 x .20 x .20	.30 x .20 x .10
CRYST. SYS.; SPACE GROUP	Monoclinic; $\text{P2}_1/\text{c}$ (#14+)	Orthorhombic; $\text{P2}_12_12_1$ (#19+)	Orthorhombic; Pnna (#52+)	Monoclinic; $\text{C2}/\text{c}$ (#15+)	Monoclinic; $\text{P2}_1/\text{c}$ (#14+)
UNIT CELL PARAMETERS	a = 16.141(9) b = 11.590(3) c = 22.863(8) $\beta = 108.95(4)^\circ$ V = 4045.3(32)	a = 12.319(4) b = 25.909(6) c = 13.132(4) V = 4191.3(45)	a = 19.502(6) b = 16.151(3) c = 14.500(7) V = 4568.1(30)	a = 15.959(5) b = 8.079(2) c = 10.732(2) $\beta = 105.42(2)^\circ$ V = 1333.9(6)	a = 12.255(4) b = 12.999(5) c = 19.873(5) $\beta = 97.45(2)^\circ$ V = 3139.5(18)
CALC. DENSITY (g cm^{-3})	1.47	1.47	1.34	1.72	2.30
OBS. DENSITY (g cm^{-3})	"	"	1.37	1.73	2.29
# REFLS. COLLECTED	7760 (quadrant)	4220 (octant)	4140 (octant)	1351 (quadrant)	6460 (quadrant)
$\sigma(I)/I$.333	.333	.333	.333	.333
# REFLS. ACCEPTED	5095	2818	2068	963	3577
2 θ MAXIMA (deg)	50.00	50.00	50.00	50.00	50.00
RANGE OF SCAN RATE (deg/min)	7.32 - 29.30	3.45 - 29.30	7.32 - 29.30	4.88 - 29.30	4.88 - 29.30
SCAN WIDTH (deg)	2.0	2.0	2.0	2.0	2.0
STANDARD REFLS.	006;040;400	400;060;006	400;080;008	10 0 0;060;008	600; 040;008
METALS PER UNIT CELL	16	16	8	4	12
FINAL R	0.081	0.056	0.083	0.038	0.065
FINAL R_w	0.095	0.049	0.093	0.040	0.078

Table 3. (Continued).

	Cu ₂ (Dapac)(OAc)	Cu ₂ (Dapsa)(OAc)·2 CH ₃ CN	Cu ₂ (Dapsa)(OAc)·CH ₃ OH	Cu ₂ (Dapsa)(OAc)	Cu(DapsaH)·CH ₃ CN
COLOR	dk. blue	dk. green	dk. green	dk. green	olive green
APPROX. SIZE (mm)	.80 x .50 x .20	.50 x .30 x .30	.50 x .40 x .20	.50 x .40 x .10	.40 x .20 x .20
CRYST. SYS.; SPACE GROUP	Monoclinic; P2 ₁ /n ^Δ	Monoclinic; C2/c (#15 [†])	Orthorhombic; Pbca (#61 [†])	Monoclinic; P2 ₁ /c (#14 [†])	Monoclinic P2 ₁ /c (#14 [†])
UNIT CELL PARAMETERS	a = 11.980(6) b = 12.216(3) c = 12.259(9) β = 104.54(5) [°] V = 1736.5(15)	a = 19.075(4) b = 10.549(2) c = 11.741(3) β = 94.04(2) [°] V = 2356.6(8)	a = 9.707(2) b = 18.153(3) c = 22.572(9) V = 3977.2(20)	a = 17.968(3) b = 20.731(4) c = 9.826(1) β = 95.44(1) V = 3643.6(9)	a = 12.541(9) b = 18.394(8) c = 7.747(7) β = 91.16(7) [°] V = 1786.7(22)
CALC. DENSITY (g cm ⁻³)	1.67	1.59	1.72	1.75	1.49
OBS. DENSITY (g cm ⁻³)	1.65	α	1.71	1.73	α
# REFLS. COLLECTED	3395 (quadrant)	2315 (quadrant)	3914 (octant)	7088 (quadrant)	3509 (quadrant)
σ(I)/I	.333	.333	.333	.333	.286
# REFLS. ACCEPTED	2561	1704	2203	4025	954
2θ MAXIMA (deg)	50.00	50.00	50.00	50.00	50.00
RANGE OF SCAN RATE (deg/min)	3.32 - 29.30	3.32 - 29.30	2.02 - 29.30	3.91 - 29.30	4.88 - 29.30
SCAN WIDTH (deg)	2.0	2.0	2.0	2.0	2.0
STANDARD REFLS.	400;060;004	008;040;600	400;060;008	400;060;002	300;040;011
METAL CENTERS PER CELL	8	8	16	16	4
* FINAL R	0.041	0.050	0.054	0.066	0.078
FINAL R _w	0.043	0.053	0.047	0.065	0.061

^Δ Non-standard space group setting.

[†] "International Tables for X-ray Crystallography", Vol. I, Kynoch Press, Birmingham, England, 1952.

α Rapid crystalline decomposition prevented density determination.

Throughout this thesis all numbers in parenthesis indicate estimated standard deviations in the last significant digit.

Solution, Refinement and Description of Structures

The observed (FO) and calculated (FC) structure factors are listed in the appendix (Tables A - J) followed by the atomic positional and thermal parameters for each structure (Tables K - T).

R and R_w values for each complex at various stages of refinement are presented in Table 4. The initial residual represents the R value which resulted from least squares refinement of the atoms found in the Patterson synthesis (or E-map where direct methods were used). Further isotropic refinement of all non-hydrogen atoms located in successive Fourier calculations lead to the residuals shown in the third column of Table 4.

[Cu(EIA)]₄·C₄H₉OH

The structure of the epoxy coated blue crystal was solved with little difficulty after locating from the Patterson synthesis the four copper atoms in the asymmetric unit. With a non-improving residual value of approximately 0.11 (coppers oxygens and nitrogens anisotropically refined) a solvent molecule of 2-butanol was fit to the

Table 4. Number of Atoms in the Asymmetric Unit, 2 θ Range of the Reflection Array, NO / NV and Residual Index Values (R and R_w) at Various Stages of Refinement for the Complexes Reported in this Thesis.

COMPOUND	ATOMS LOC. FROM PATTERSON SYN.	INITIAL R INITIAL R _w	NON-HYDROGEN ATOMS ISOTROPIC R, R _w	FINAL R FINAL R _w	# ATOMS LOC. IN ASYM. UNIT	2 θ RANGE OF REFLECTION ARRAY	NO / NV
[Cu(ETA)] ₄ ·C ₄ H ₉ OH	4 Coppers 4 Oxygens	0.287 0.340	0.130 0.146	0.081 0.095	49	7.03 - 23.82	5096 / 277
[Ni(ETA)(CH ₃ OH)] ₄	4 Nickels*	0.293 0.323	0.084 0.084	0.056 0.049	52	3.66 - 14.96	2818 / 229
Fe ₂ (DSALZ) ₃ ·C ₃ H ₆ O	1 Iron*	0.441 0.465	0.111 0.097	0.083 0.093	31	4.19 - 20.28	2068 / 226
[Co(Dapo)(DapoH)]Cl ₂ ·2H ₂ O	1 Cobalt 1 Oxygen 2 Nitrogens	0.492 0.480	0.058 0.063	0.038 0.040	15	5.69 - 23.33	963 / 97
[Cu ₃ (Dapo) ₂ (DapoH) ₂]I ₄ ·CH ₃ OH	3 Iodines*	0.458 0.520	0.156 0.178	0.065 0.078	52	9.31 - 25.30	3577 / 228
Cu ₂ (Dapac)(OAc)	2 Coppers	0.337 0.354	0.078 0.086	0.041 0.043	31	4.23 - 21.19	2560 / 238
Cu ₂ (Dapac)(OAc)·2CH ₃ CN	1 Copper	0.373 0.398	0.098 0.124	0.050 0.053	26	4.26 - 23.14	1704 / 177
Cu ₂ (Dapac)(OAc)·CH ₃ OH	2 Coppers	0.492 0.497	0.117 0.125	0.054 0.047	45	3.57 - 22.91	2203 / 176
Cu ₂ (Dapac)(OAc)	2 Coppers	0.566 0.598	0.105 0.107	0.066 0.065	56	6.29 - 22.54	4025 / 315
Cu(DapacH)·CH ₃ CN	1 Copper	0.352 0.379	0.095 0.069	0.078 0.061	26	3.30 - 14.30	954 / 110

* Located using light atom methods.

five highest peaks (avg $1.5 \text{ e}/\text{\AA}^3$) in the electron density map. Final refinement, including these additional atoms, reduced the residual to 0.09.

Tables A and K of the appendix contain the structure factors and the atomic parameters, respectively. Table 5 in this chapter lists some selected bond distances and angles for this complex.

The complex crystallizes with four discrete, tetrameric "cubane" moieties per unit cell (Figure 12). The idealized local symmetry of each copper is square pyramidal. Two oxygens of the tridentate ligand EIA occupy two trans basal positions with the nitrogen chelating to a third basal position. The remaining basal site and the apical position are filled by the ethanolamine alkoxide oxygens of two adjacent EIA ligands. The "cubane" unit is composed of four tetrahedrally disposed coppers with a tetrahedron of oxygen atoms acting as bridges. An interesting structural aspect of this distorted cube is that it assumes a tub conformation. That is, there are two pairs of long, mutually perpendicular copper-oxygen bonds ($2.37 - 2.43 \text{ \AA}$) while the remaining eight copper-oxygen bonds of the cube are comparatively shorter ($1.94 - 1.98 \text{ \AA}$). The tub-like conformation can be easily seen in Figure 12, where the longer bonds are drawn as unfilled stick bonds.

Table 5. Selected Interatomic Distances (Å) and Angles (deg)
for $[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$.

ATOMS	n=	1	2	3	4	AVG
DISTANCES						
O(n1)-C(n1)		1.45(1)	1.44(1)	1.43(2)	1.43(2)	1.44(1)
C(n1)-C(n2)		1.51(2)	1.53(2)	1.53(2)	1.54(2)	1.53(1)
C(n2)-N(n)		1.49(2)	1.51(2)	1.50(2)	1.47(2)	1.49(2)
N(n)-C(n4)		1.27(2)	1.32(2)	1.33(2)	1.34(2)	1.32(3)
C(n3)-C(n4)		1.55(2)	1.56(2)	1.51(2)	1.52(2)	1.54(2)
C(n4)-C(n5)		1.42(2)	1.43(2)	1.42(2)	1.42(2)	1.42(1)
C(n5)-C(n6)		1.39(2)	1.37(2)	1.32(2)	1.35(2)	1.36(3)
C(n6)-C(n7)		1.52(2)	1.61(2)	1.57(2)	1.57(2)	1.57(4)
C(n6)-O(n2)		1.24(2)	1.28(2)	1.31(2)	1.32(2)	1.29(3)
Cu(1)-Cu(n)		*	3.146(2)	3.109(3)	3.314(3)	*
Cu(2)-Cu(n)		*	*	3.314(3)	3.148(3)	*
Cu(3)-Cu(n)		*	*	*	3.131(3)	*
Cu(1)-O(n1)		1.962(8)	1.946(8)	*	2.425(8)	*
Cu(2)-O(n1)		*	1.975(8)	2.429(8)	1.976(8)	*
Cu(3)-O(n1)		1.955(8)	2.367(8)	1.974(8)	*	*
Cu(4)-O(n1)		2.430(8)	*	1.941(8)	1.959(8)	*
Cu(n)-O(n2)		1.898(9)	1.923(8)	1.920(9)	1.93(1)	*
Cu(n)-N(n)		1.94(1)	1.919(9)	1.91(1)	1.93(1)	*

ATOMS	n=	1	2	3	4	AVG
ANGLES						
Cu(n)-O(n1)-C(n1)		108.8(7)	109.8(7)	108.8(7)	110.6(7)	109.5(8)
Cu(n)-O(n2)-C(n6)		124.2(9)	122(1)	131(1)	120(1)	124(4)
Cu(n)-N(n)-C(n2)		110.5(8)	113.2(7)	113.5(8)	114.7(8)	113.0(15)
Cu(n)-N(n)-C(n4)		126(1)	125.7(9)	126.4(9)	124(1)	125.5(9)
O(n1)-Cu(n)-O(n2)		178.8(4)	180.0(3)	179.2(4)	177.1(4)	178.8(10)
O(n1)-Cu(n)-N(n)		86.3(4)	84.1(4)	85.0(4)	83.2(4)	84.7(11)
O(n2)-Cu(n)-N(n)		94.4(4)	96.0(4)	94.9(4)	96.2(5)	95.4(8)
O(n1)-C(n1)-C(n2)		109(1)	107(1)	109(1)	107(1)	108(1)
O(n2)-C(n6)-C(n5)		128(1)	129(2)	131(1)	127(2)	129(2)
O(n2)-C(n6)-C(n7)		116(1)	113(1)	110(1)	111(2)	113(2)
C(n2)-N(n)-C(n4)		124(1)	121(1)	120(1)	120(1)	121(2)
N(n)-C(n2)-C(n1)		110(1)	106(1)	107(1)	107(1)	108(2)
N(n)-C(n4)-C(n3)		119(1)	122(1)	122(1)	121(1)	121(1)
N(n)-C(n4)-C(n5)		124(1)	122(1)	122(1)	121(1)	122(1)
C(n3)-C(n4)-C(n5)		117(1)	116(1)	116(1)	119(1)	117(1)
C(n4)-C(n5)-C(n6)		124(1)	125(2)	125(1)	128(2)	126(2)
C(n5)-C(n6)-C(n7)		115(1)	118(2)	120(1)	122(2)	119(3)

Table 5. (Continued).

ATOMS	ANGLE	ATOMS	ANGLE
O11 - Cu1 - O41	81.9(3)	Cu1 - O11 - Cu3	105.1(4)
O11 - Cu1 - O21	86.3(3)	Cu1 - O11 - Cu4	97.4(3)
O21 - Cu1 - O41	75.2(3)	Cu3 - O11 - Cu4	90.5(3)
N1 - Cu1 - O21	165.7(4)	Cu3 - O11 - C11	125.1(7)
N1 - Cu1 - O41	115.9(4)	Cu4 - O11 - C11	125.4(7)
O21 - Cu2 - O31	81.0(3)	Cu1 - O21 - Cu2	106.7(3)
O21 - Cu2 - O41	86.0(3)	Cu1 - O21 - Cu3	91.7(3)
O31 - Cu2 - O41	74.2(3)	Cu2 - O21 - Cu3	98.3(3)
N2 - Cu2 - O31	112.3(4)	Cu1 - O21 - C21	123.8(7)
N2 - Cu2 - O41	167.0(4)	Cu3 - O21 - C21	122.6(7)
O31 - Cu3 - O11	86.9(3)	Cu2 - O31 - Cu3	96.4(3)
O31 - Cu3 - O21	82.7(3)	Cu2 - O31 - Cu4	91.5(3)
O21 - Cu3 - O11	75.8(3)	Cu3 - O31 - Cu4	106.2(4)
N3 - Cu3 - O11	168.0(4)	Cu4 - O31 - C31	126.4(7)
N3 - Cu3 - O21	111.9(3)	Cu2 - O31 - C31	122.8(7)
O41 - Cu4 - O11	81.9(3)	Cu1 - O41 - Cu2	90.7(3)
O41 - Cu4 - O31	86.9(3)	Cu1 - O41 - Cu4	97.6(3)
O11 - Cu4 - O31	75.5(3)	Cu2 - O41 - Cu4	106.2(4)
N4 - Cu4 - O11	105.1(4)	Cu1 - O41 - C41	119.6(7)
N4 - Cu4 - O31	169.9(4)	Cu2 - O41 - C41	127.2(7)

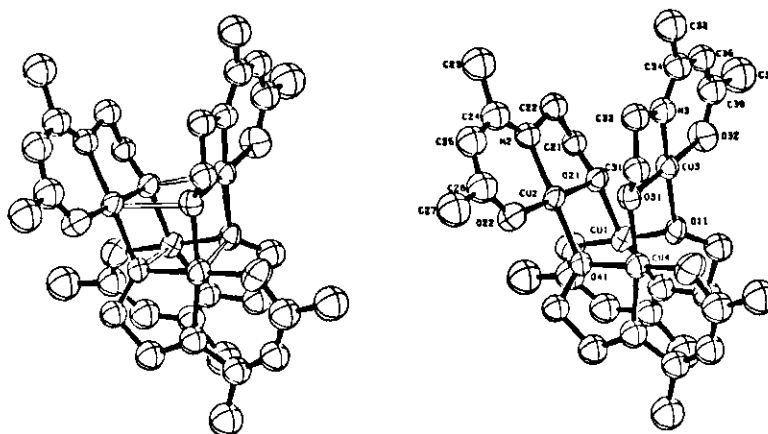
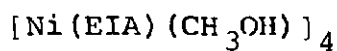


Figure 12. Stereoview of the Tetramer $[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$. Solvent Molecule and Numbering Scheme for the #1 and #4 Ligands Omitted for Clarity. Unfilled Stick Bonds Represent the Longer Bonds in the Cu_4O_4 Cube Moiety.

Although it is not crystallographically necessary, the bond distances and angles for analogous parts of the tetramer are approximately equivalent. This is evident from the average bond distances and angles and their standard deviation values which are listed in Table 5.



The structure was solved by direct methods using the program MULTAN; the program was allowed to choose

origin-defining reflections and the correct solution was apparent from the Figure-of Merit index. Positions of all the nickel atoms were obtained from the initial E-map and all other non-hydrogen atoms were located in successive difference Fourier calculations.

Tables B and L in the appendix contain the structure factors and the atomic parameters, respectively, for the structure. Table 6 in this chapter lists the selected bond distances and angles for the final structure.

The structure consists of discrete, tetrameric, cubane-like molecules. A stereoview of the molecule is presented in Figure 13.

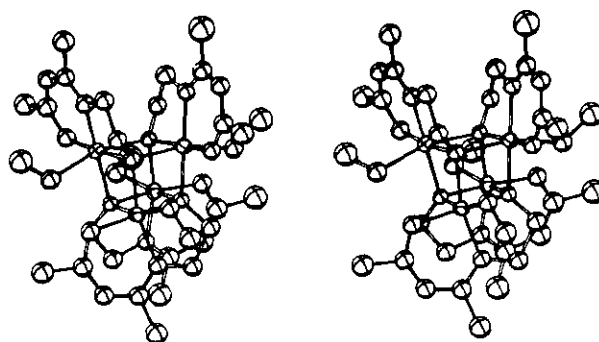


Figure 13. Stereoview of the Cubane Complex $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_4$.

Although each nickel atom of the tetramer is crystallographically independent, the coordination arrangement around each is very similar. Each nickel atom is coordinated to an EIA ligand through the nitrogen and

Table 6. Selected Interatomic Distances (Å) and Angles (deg)
for $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_4$.

Atoms	n =	1	2	3	4	Avg.
Interatomic Distances						
Ni(n)-O(n1)		2.051(8)	2.032(7)	2.030(7)	2.020(7)	2.033(11)
Ni(n)-O(n2)		1.978(8)	1.998(8)	1.996(7)	1.991(8)	1.991(8)
Ni(n)-N(n)		1.93(1)	1.98(1)	1.98(1)	1.99(1)	1.97(2)
Ni(n)-O(n3)		2.17(8)	2.245(8)	2.215(8)	2.186(8)	2.21(3)
O(n1)-C(n1)		1.45(1)	1.45(1)	1.42(1)	1.43(1)	1.44(1)
O(n2)-C(n6)		1.32(1)	1.31(1)	1.28(1)	1.32(1)	1.31(2)
O(n3)-C(n8)		1.46(2)	1.47(2)	1.44(2)	1.45(2)	1.45(1)
N(n)-C(n2)		1.49(1)	1.46(1)	1.46(1)	1.45(1)	1.47(2)
N(n)-C(n4)		1.29(1)	1.34(1)	1.33(1)	1.30(1)	1.32(2)
C(n1)-C(n2)		1.57(2)	1.54(2)	1.60(2)	1.50(2)	1.55(4)
C(n4)-C(n5)		1.40(2)	1.41(2)	1.38(2)	1.46(2)	1.41(3)
C(n5)-C(n6)		1.37(2)	1.32(2)	1.42(2)	1.31(2)	1.36(4)
C(n3)-C(n4)		1.56(2)	1.54(2)	1.54(2)	1.55(2)	1.55(1)
C(n6)-C(n7)		1.50(2)	1.58(2)	1.51(2)	1.56(2)	1.54(3)
Ni(1)-Ni(n)			3.052(3)	3.210(2)	3.056(2)	
Ni(2)-Ni(n)				3.065(2)	3.198(2)	
Ni(3)-Ni(n)					3.056(3)	
Atoms	n, n' =	1,4	2,1	3,2	4,3	Avg.
Ni(n)-O(n'1)		2.054(7)	2.032(7)	2.023(7)	2.055(7)	2.037(13)
Ni(n)-O(n''1)		2.122(7)	2.112(7)	2.115(7)	2.130(7)	2.120(7)
Atoms	n =	1	2	3	4	Avg.
Angles About Ni						
O(n2)-Ni(n)-O(n3)		93.1(3)	93.5(3)	95.2(3)	74.8(4)	93.9(9)
O(n2)-Ni(n)-N(n)		93.9(3)	94.5(4)	93.5(3)	94.4(4)	94.1(4)
O(n3)-Ni(n)-N(n)		92.8(3)	70.5(4)	90.7(3)	89.3(4)	91(1)
O(n1)-Ni(n)-O(n3)		94.5(3)	94.4(3)	93.1(3)	113.3(3)	94.0(6)
O(n1)-Ni(n)-O(n2)		172.1(3)	170.8(3)	171.4(3)	171.6(3)	171.5(5)
O(n1)-Ni(n)-N(n)		83.8(3)	83.7(3)	84.4(4)	83.8(3)	83.9(3)

Table 6. (Continued).

Atoms	n, n' =	1,4	2,1	3,2	4,3	Avg.
N(n)-Ni(n)-O(n'1)		165.8(3)	164.1(4)	166.1(3)	165.6(3)	165.4(8)
O(n2)-Ni(n)-O(n'1)		99.3(3)	99.8(3)	98.5(3)	98.3(3)	99.0(6)
O(n1)-Ni(n)-O(n'1)		83.8(3)	83.3(3)	84.7(3)	84.6(3)	84.1(6)
O(n3)-Ni(n)-O(n'1)		81.3(3)	101.6(3)	81.3(3)	87.6(4)	83(3)
Atoms	n, n', n'' =	1,4,3	2,1,4	3,2,1	4,3,2	Avg.
O(n'1)-Ni(n)-O(n''1)		82.9(3)	82.8(3)	81.5(3)	81.5(3)	82.0(5)
O(n1)-Ni(n)-O(n''1)		78.6(3)	79.1(3)	79.3(3)	79.0(3)	79.0(3)
O(n3)-Ni(n)-O(n''1)		162.6(3)	171.8(3)	161.8(3)	162.7(3)	165(4)
N(n)-Ni(n)-O(n''1)		102.2(3)	103.5(3)	105.0(3)	104.5(4)	104(1)
O(n2)-Ni(n)-O(n''1)		94.6(3)	92.5(3)	93.2(3)	93.5(3)	93.5(8)
Atoms	n =	1	2	3	4	Avg.
Ligand Angles						
Ni(n)-O(n1)-C(n1)		107.8(6)	107.3(6)	108.9(6)	107.6(5)	107.9(6)
O(n1)-C(n1)-C(n2)		109.3(9)	109.8(9)	108.9(9)	111.2(8)	109.8(9)
C(n1)-C(n2)-N(n)		109.1(9)	109.3(9)	110(1)	111(1)	110(1)
N(n)-C(n4)-C(n3)		117(1)	118(1)	120(1)	119(1)	118(1)
N(n)-C(n4)-C(n5)		122(1)	123(1)	122(1)	123(1)	122(1)
C(n4)-C(n5)-C(n6)		131(1)	129(1)	130(1)	128(1)	130(1)
C(n5)-C(n6)-C(n7)		123(1)	120(1)	121(1)	119(1)	121(1)
C(n5)-C(n6)-O(n2)		123(1)	129(1)	124(1)	127(1)	126(2)
C(n6)-O(n2)-Ni(n)		124.1(7)	121.3(7)	124.5(7)	122.5(8)	123(1)
Ni(n)-O(n3)-C(n8)		126.3(8)	127.2(8)	129.2(7)	120.6(8)	126(3)

two oxygen atoms of the ligand. In addition, each nickel atom is coordinated to methanol oxygen and to the alkoxide oxygen atoms, O1, of two adjacent ligands. The numbering system employed is identical to that used in the complex $[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$ with the additional methanol molecule of the nickel structure labeled as O(n3) and C(n8). The coordination about each nickel is tetragonally-distorted octahedron. The three donor atoms of the coordinated ligand and one bridging alkoxide from an adjacent ligand form the basal plane with the shorter distances (1.93 - 2.06 Å). The methanol oxygen and the other alkoxide oxygen occupy the axial positions with the longer distances (2.11 - 2.25 Å). The methanol coordinated to Ni(2) is bent toward the nitrogen (N2) to give an angle of 70.4 degrees compared to the average angle of 91.0 degrees. The methanol coordinated to Ni(4) is bent toward O2 to give an angle of 74.8 compared to an average angle of 93.9 degrees for the other three groups.

$\text{Fe}_2 (\text{DSALZ})_3 \cdot \text{C}_3\text{H}_6\text{O}$

The structure was solved by direct methods using the program MULTAN; the program was allowed to choose origin-defining reflections and the correct solution was apparent from the Figure-of-Merit index. The iron(III) atom was located from the E-map and all other non-hydrogen

atoms were found in the successive difference Fourier calculations.

Table C and M in the appendix contain the structure factors and the atomic parameters from the final refinement, respectively. Table 7 presents the selected bond distances and angles for the complex.

$\text{Fe}_2(\text{DSALZ})_3 \cdot \text{C}_3\text{H}_6\text{O}$ crystallizes as discrete dimers. The asymmetric unit contains one half of a dinuclear unit; the numbering system for the molecule is shown in Figure 14.

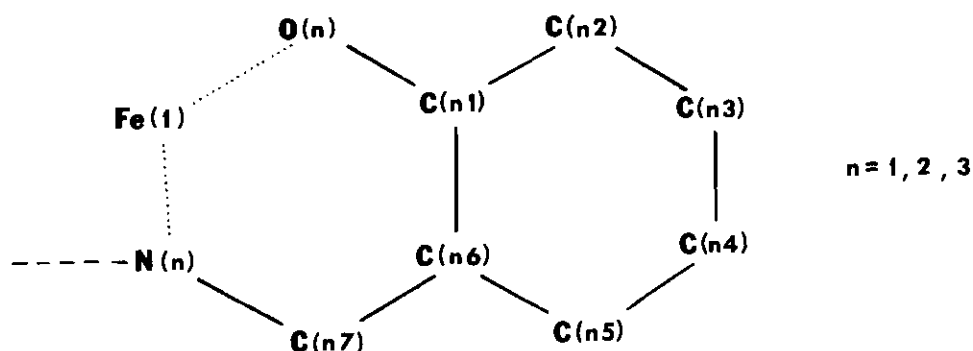


Figure 14. Numbering Scheme for $\text{Fe}_2(\text{DSALZ})_3$.

The two-fold symmetry imposed by the space group Pnna generates the remaining portion of the dimer (Figure 15). The iron atom is octahedrally coordinated to three oxygens and three nitrogens in a facial manner. The two octahedra

Table 7. Selected Bond Distances (Å) and Angles (deg) for the Complex $\text{Fe}_2(\text{DSALZ})_3 \cdot \text{C}_3\text{H}_6\text{O}$.

ATOMS	n=	1	2	3
DISTANCES				
Fe(1)-O(n)		1.906(8)	1.907(9)	1.906(7)
Fe(1)-N(n)		2.189(9)	2.17(1)	2.188(8)
O(n)-C(n1)		1.32(2)	1.27(2)	1.30(1)
N(n)-C(n7)		1.32(1)	1.30(2)	1.30(1)
C(n1)-C(n2)		1.43(2)	1.42(2)	1.42(1)
C(n2)-C(n3)		1.36(2)	1.39(2)	1.38(2)
C(n3)-C(n4)		1.37(3)	1.34(2)	1.36(2)
C(n4)-C(n5)		1.40(2)	1.43(2)	1.40(2)
C(n5)-C(n6)		1.46(2)	1.42(2)	1.38(2)
C(n6)-C(n7)		1.45(2)	1.47(2)	1.43(2)
C(n6)-C(n1)		1.37(2)	1.44(2)	1.42(1)
N(n)-N(n')		*	*	1.39(1)
Fe(n)-Fe(n')		3.944(4)	*	*
ANGLES				
Fe(1)-O(n)-C(n1)		135.9(9)	136.9(9)	133.3(7)
Fe(1)-N(n)-C(n7)		127.2(8)	127.8(8)	124.7(7)
O(n)-C(n1)-C(n2)		118(1)	120(2)	119(1)
O(n)-C(n1)-C(n6)		123(1)	122(1)	123(1)
N(n)-C(n7)-C(n6)		122(1)	122(1)	126(1)
C(n6)-C(n1)-C(n2)		119(1)	117(2)	118.5(9)
C(n1)-C(n2)-C(n3)		120(2)	120(2)	121(1)
C(n2)-C(n3)-C(n4)		123(2)	124(3)	121(1)
C(n3)-C(n4)-C(n5)		120(1)	119(2)	119(2)
C(n4)-C(n5)-C(n6)		117(2)	119(2)	118(2)
C(n5)-C(n6)-C(n7)		112(1)	115(2)	116(1)
C(n5)-C(n6)-C(n1)		122(1)	121(1)	121(1)
C(n1)-C(n6)-C(n7)		126(1)	124(1)	123(1)

All atom parameters given for atoms within asymmetric unit.

Table 7. (Continued).

ATOMS	ANGLE	ATOMS	ANGLE
N(2')-Fe(1)-O(3)	168.5(3)	O(1)-Fe(1)-O(3)	100.1(4)
N(3)-Fe(1)-O(1)	168.4(3)	O(1)-Fe(1)-N(1)	84.7(4)
N(1)-Fe(1)-O(2')	169.7(4)	N(3)-Fe(1)-N(2')	83.6(3)
O(2')-Fe(1)-O(1)	98.4(4)	N(3)-Fe(1)-O(3)	85.0(3)
O(2')-Fe(1)-N(2')	84.5(4)	N(3)-Fe(1)-N(1)	84.6(3)
O(2')-Fe(1)-O(3)	94.9(4)	N(1)-Fe(1)-N(2')	85.6(4)
O(2')-Fe(1)-N(3)	91.5(4)	N(1)-Fe(1)-O(3)	94.2(4)
O(1)-Fe(1)-N(2')	91.3(4)		

X related to X' by the symmetry transformation: $x, 1/2-y, 1/2-z$

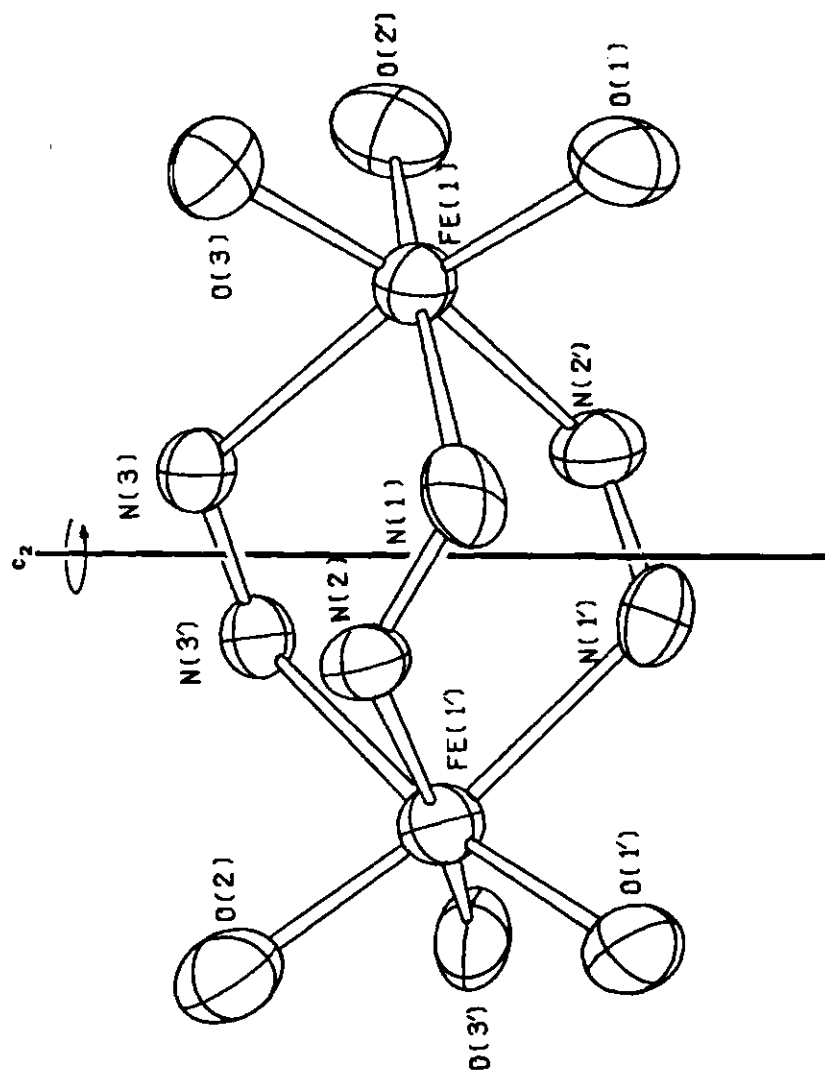
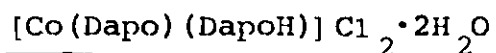


Figure 15. A View of the Dimer $\text{Fe}_2(\text{DSALZ})_3$ Omitting the Acetone Molecule of Solvation. Atom X Related to X' by Rotation Through the Two-fold Axis (Heavy Line Approximately Parallel to the Plane of the Paper).

composing the dimer (Fe(1) - Fe(1') dist. = 3.944 Å) do not share a common face but rather are separated by the distance of the N-N azine bond (1.39 Å). The site midway between the Fe(1) and Fe(1') atoms assumes a trigonal prismatic geometry with respect to the two faces. There is an average deviation of 24 degrees away from the eclipsing of the nitrogen atoms. Each crystallographically independent ligand has similar structural parameters.

Two complete data sets were collected on separate crystals in an effort to satisfactorily refine this structure. Although the second specimen gave much stronger diffraction, the structure did not refine below an R value of 0.12. Based on the analytical results and several peaks in the difference fourier (range 1.1 - 1.8 e/Å³), an acetone molecule positioned on the two-fold axis was found to best fit the observed data. Disorder problems prevented sharp refinement of the solvent atoms so the fractional coordinates and temperature factors of these atoms were input at fixed values.

The magnetic moment of this complex shows a slight decrease (5.5 - 5.1 BM) with temperature (298 - 98 °K); the values are in the normal range for a high spin d⁵ complex.



Due to the number of molecules in the unit cell, the position of the cobalt atom in the asymmetric unit was fixed at the special position (.00, .00, .00). The successive difference Fourier calculations revealed the positions of the remaining non-hydrogen atoms and also one hydrogen atom (HBND). Other hydrogens were located geometrically (C - H dist.= .95) and included in the final refinement, varying their positional parameters and setting their temperature factors at 5.0.

Tables D and N in the appendix contain the structure factors and atomic parameters, respectively. Table 8 lists the selected interatomic distances and angles for the complex.

Local geometry around the cobalt atom is octahedral with a slight trigonal distortion due to the chelation of the tridentate ligand. The oxygen atoms of the Dapo and DapoH ligands are trans to each other and, since the cobalt atom is on an inversion center, the bond distances of the cobalt to the protonated and deprotonated oxygens are crystallographically equivalent (as are the analogous cobalt-nitrogen bond distances).

The gross crystal structure revealed octahedral units interacting through hydrogen bonding along the crystallographic c-axis, to form infinite linear chains

Table 8. Selected Interatomic Distances (Å) and Angles (deg) for
 $[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$.^{a,b}

ATOMS	DIST.	ATOMS	DIST.
Co1 - O1	1.901(3)	N2 - C2	1.500(5)
Co1 - N1	1.963(4)	C2 - C3	1.514(6)
Co1 - N2	1.967(3)	C1 - C3	1.517(6)
O1 - C3	1.438(5)	O1 - O1''	2.420(6)
N1 - C1	1.496(5)	O1 - HBND	1.01(13)
HBND - HBND''	0.60(20)	O1 - HBND''	1.46(13)

ATOMS	ANGLE	ATOMS	ANGLE
O1 - Co1 - N2	86.7(1)	Co1 - N1 - C1	107.3(2)
O1 - Co1 - N1	86.7(1)	Co1 - N1 - C2	107.3(2)
N1 - Co1 - N2	85.7(1)	O1 - C3 - C2	104.9(3)
O1 - Co1 - N1'	93.3(1)	O1 - C3 - C1	107.1(3)
O1 - Co1 - N2'	95.9(1)	C3 - C1 - N1	107.1(3)
N1 - Co1 - N2'	94.3(1)	C3 - C2 - N2	107.8(3)
Co1 - O1 - C3	101.4(2)	O1 - HBND - O1''	156.5(5)

a X related to X' by inversion.

b X related to X'' by the transformation; $-x, y, 1/2-z$.

(Figure 16). The distance between the oxygens involved in hydrogen bonding (O(1) and O(1'')) is 2.42 Å. Although the hydrogen (HBND) is required by symmetry to be on a two-fold axis and to be equidistant from the oxygens, when the positional parameters of this hydrogen were refined, the highest point of electron density refined off of the two fold axis. This implies that the hydrogen is disordered in the structure.



The positions of the three iodine atoms were obtained by using the program MULTAN; the program was allowed to choose origin-defining reflections and the correct solution was apparent from the Figure-of-Merit index. The remaining non-hydrogen atoms were located in successive difference Fourier calculations.

Tables E and O in the appendix list the structure factors and atomic parameters, respectively. Table 9 contains the selected interatomic distances and angles for the trimer.

The compound crystallizes in discrete, trimeric units. The trinuclear cation (Figure 17) contains a central, four coordinate copper(II) chelated to the two deprotonated ligands through the oxygen and one nitrogen of each ligand with a cis arrangement. Each of the deprotonated ligands is

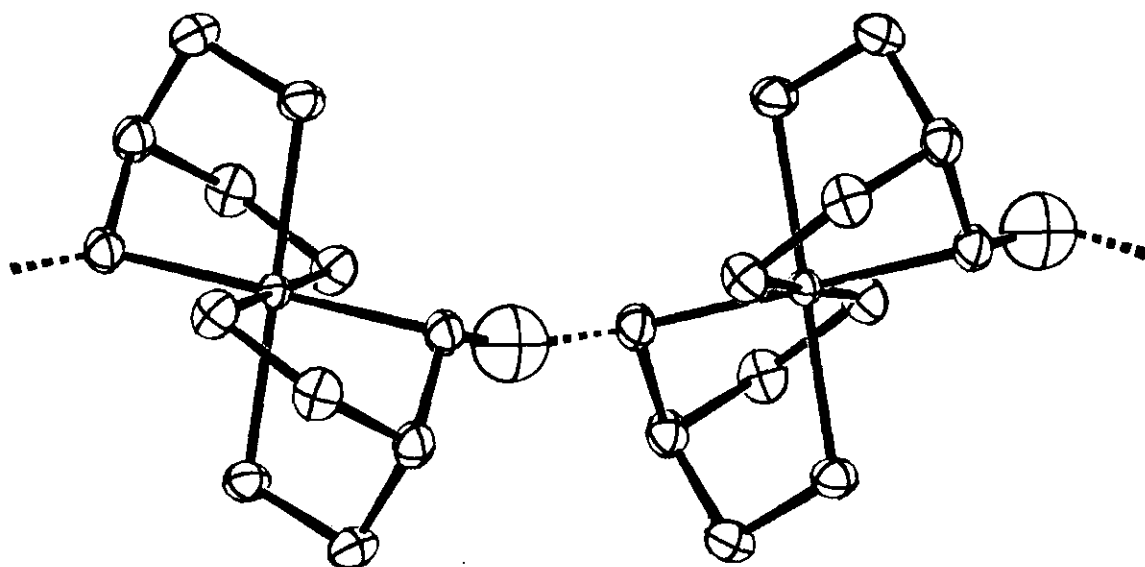


Figure 16. Molecular Structure of the Cation $[\text{Co}(\text{Dapo})(\text{DapoH})]^{2+}$. Dashed Bonds Indicate Intermolecular Linear Chain H-bonding.

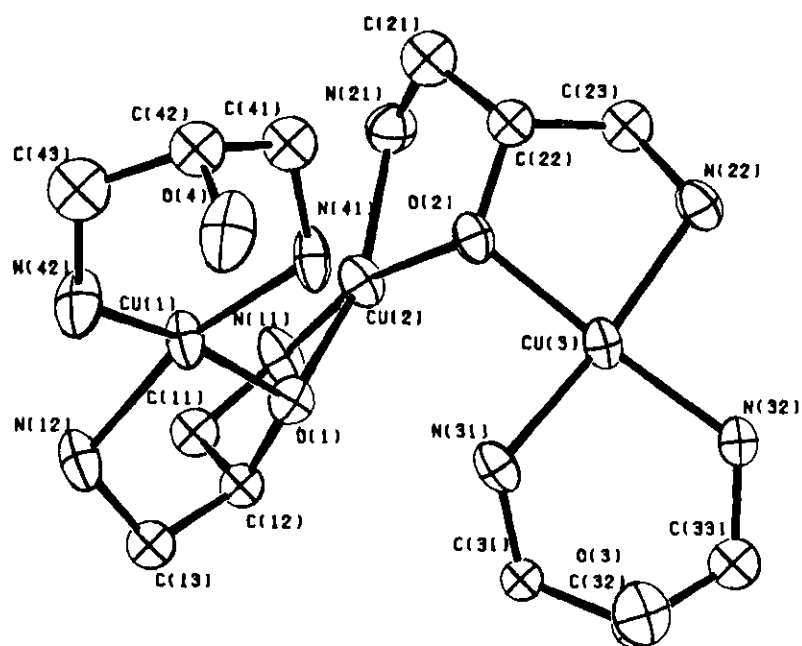


Figure 17. A View of the Trinuclear Cation of the Complex Whose Formula is $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$. Hydrogen Atoms Omitted for Clarity.

also coordinated to a terminal copper(II) through the oxygen (bridging) and the remaining nitrogen. The square planar coordination of each terminal copper (II) is completed by the two nitrogens of a neutral ligand; the alcohol groups of the neutral ligand are not coordinated. The Cu1 - Cu2 - Cu3 angle is 95.8 degrees. Although there is no crystallographic symmetry imposed on the molecule, analogous bond distances and angles within the molecule are equivalent (Table 9).

The least squares plane analyses (Table 10.) for the trimeric species revealed that of the three metal coordination spheres, the central one is most distorted from planarity. However, a terminal copper(II), Cu(1), lies farthest from the best fit plane (0.213 Å) compared to Cu(2) and Cu(3) lying only 0.022 Å and 0.099 Å, respectively, from the plane.

The results of the variable temperature magnetic study for the trimer are presented in Table 11.

Cu₂(Dapac) (OAc)

The two copper(II) atoms in the asymmetric unit were located via a Patterson synthesis. The remaining non-hydrogen atoms were found from successive difference Fourier calculations. All hydrogen atoms were located geometrically (C - H dist = 0.95 Å) and their parameters refined, setting the temperature factors constant at 5.0.

Table 9. Selected Interatomic Distances (Å) and Angles (deg) for $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$.

ATOMS	DIST.	ATOMS	DIST.
Cu(1) - Cu(2)	3.368(4)	N(11) - C(11)	1.46(2)
Cu(2) - Cu(3)	3.394(3)	N(12) - C(13)	1.48(3)
Cu(1) - O(1)	2.02(1)	N(21) - C(21)	1.47(3)
Cu(1) - N(12)	2.02(2)	N(22) - C(23)	1.49(3)
Cu(1) - N(41)	2.03(2)	N(31) - C(31)	1.44(2)
Cu(1) - N(42)	2.05(2)	N(32) - C(33)	1.48(3)
Cu(2) - O(1)	1.99(1)	N(41) - C(41)	1.50(3)
Cu(2) - O(2)	1.96(1)	N(42) - C(43)	1.42(3)
Cu(2) - N(11)	2.00(2)	C(11) - C(12)	1.54(3)
Cu(2) - N(21)	2.01(2)	C(12) - C(13)	1.53(3)
Cu(3) - O(2)	2.00(1)	C(21) - C(22)	1.50(3)
Cu(3) - N(22)	2.03(2)	C(22) - C(23)	1.53(3)
Cu(3) - N(31)	2.02(2)	C(31) - C(32)	1.52(3)
Cu(3) - N(32)	2.03(2)	C(32) - C(33)	1.53(3)
O(1) - C(12)	1.41(2)	C(41) - C(42)	1.54(3)
O(2) - C(22)	1.45(2)	C(42) - C(43)	1.59(3)
O(3) - C(32)	1.45(2)	OSOLV - CSOLV	1.33(3)
O(4) - C(42)	1.45(3)		

ATOMS	ANGLE	ATOMS	ANGLE
O(1)-Cu(1)-N(41)	92.3(6)	O(1)-C(12)-C(11)	109(2)
O(1)-Cu(1)-N(12)	83.3(6)	O(1)-C(12)-C(13)	109(2)
N(12)-Cu(1)-N(42)	92.3(7)	N(11)-C(11)-C(12)	109(2)
N(41)-Cu(1)-N(42)	89.7(7)	N(12)-C(13)-C(12)	109(2)
O(1)-Cu(2)-O(2)	94.0(5)	C(11)-C(12)-C(13)	112(2)
O(1)-Cu(2)-N(11)	86.1(6)	Cu(2)-O(2)-Cu(3)	118.2(6)
O(2)-Cu(2)-N(21)	85.7(6)	Cu(2)-O(2)-C(22)	112(1)
N(11)-Cu(2)-N(21)	99.8(7)	Cu(2)-N(21)-C(21)	105(1)
O(2)-Cu(3)-N(22)	84.5(6)	Cu(3)-O(2)-C(22)	112(1)
O(2)-Cu(3)-N(31)	91.4(6)	Cu(3)-N(22)-C(23)	106(1)
N(22)-Cu(3)-N(32)	92.7(6)	O(2)-C(22)-C(21)	111(2)
N(31)-Cu(3)-N(32)	91.0(7)	O(2)-C(22)-C(23)	108(2)
Cu(2)-N(11)-C(11)	107(1)	N(21)-C(21)-C(22)	110(2)
Cu(2)-O(1)-C(12)	110(1)	N(22)-C(23)-C(22)	109(2)
Cu(1)-O(1)-Cu(2)	114.4(6)	C(21)-C(22)-C(23)	111(2)
Cu(1)-O(1)-C(12)	113(1)	Cu(3)-N(31)-C(31)	116(1)
Cu(1)-N(12)-C(13)	108(1)	Cu(3)-N(32)-C(33)	120(1)

Table 9. (Continued).

ATOMS	ANGLE	ATOMS	ANGLE
O(3)-C(31)-C(32)	110(2)	Cu(1)-N(42)-C(43)	118(2)
O(3)-C(32)-C(33)	108(2)	O(4)-C(42)-C(41)	109(2)
N(31)-C(31)-C(32)	115(2)	O(4)-C(42)-C(43)	105(2)
N(32)-C(33)-C(32)	114(2)	N(41)-C(41)-C(42)	111(2)
C(31)-C(32)-C(33)	113(2)	N(42)-C(43)-C(42)	114(2)
Cu(1)-N(41)-C(41)	118(1)	C(41)-C(42)-C(43)	113(2)

Table 10. Least Squares Plane Analyses for the complex
 $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$.^{a,b}

ATOM	DEVIATION (Å)	ATOM	DEVIATION (Å)
(a) Equation of the plane involving N(21), O(2), O(1) and N(11):			
$0.8620x + 0.4658y + 0.2001z = 6.2324$			
O(1)	-0.419	N(21)	-0.235
O(2)	0.269	Cu(2)	0.022
N(11)	0.320		
(b) Equation of the plane involving O(1), N(12), N(42) and N(41):			
$-0.7866x + 0.5403y + 0.2988z = 0.8074$			
O(1)	0.097	N(42)	0.029
N(12)	-0.081	Cu(1)	0.213
N(41)	-0.073		
(c) Equation of the plane involving O(2), N(22), N(31) and N(32):			
$-0.1606x - 0.9475y + 0.2764z = -4.3711$			
O(2)	-0.046	N(32)	-0.047
N(22)	0.046	Cu(3)	-0.099
N(31)	0.049		

^aDirection cosines of the plane refer to the orthogonal axis system a, b, c.

^bAll atoms weighted at unity.

Table 11. Diamagnetic Correction (χ_{dia}), Molar Susceptibilities ($\chi_{\text{M}}^{\text{corr}}$) and Effective Moments (μ_{eff}) for the Complex $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$.

T (°K)	$\chi_{\text{M}}^{\text{corr}} \times 10^6$ cgs	μ_{eff} (BM)
$\chi_{\text{dia}} = -0.000162$		
298	1011	1.57
278	1044	1.53
258	1115	1.52
238	1172	1.50
218	1215	1.46
198	1277	1.43
178	1319	1.38
158	1395	1.33
138	1476	1.28
118	1556	1.22
98	1717	1.17

Tables F and P in the appendix contain the structure factors and atomic parameters, respectively, for the dinuclear complex. Selected bond distances and angles for the complex are listed in Table 12. In Table 13 are presented the results of the least squares plane analyses for the coordination spheres about the copper(II) atoms. The coordination sphere of Cu(1) shows larger deviations from planarity than that of Cu(2), but both are significantly distorted.

The copper(II) complex with Dapac and OAc as ligands exists as discrete, binuclear molecules in the solid state (Figure 18). The two copper(II) atoms are four coordinate and bridged by both the isopropoxide oxygen of Dapac and the oxygens (three atoms bridge) of the acetate ligand. The remaining two coordination sites on each copper(II) are filled by the alkoxide oxygens and the imine nitrogens of the pentadentate, binucleating ligand.

An interesting structural feature of the dinuclear compound is the dihedral angle between the two coordination spheres of the coppers, 123 degrees. The bent nature of the complex is discussed later with regard to the magnetic properties which it exhibits.

Variable temperature magnetic studies were undertaken and the results are listed in the first column of Table 19.

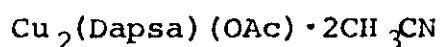


Table 12. Selected Interatomic Distances (Å) and Angles (deg)
for Cu₂(Dapac)(OAc).

ATOMS	DIST.	ATOMS	DIST.
Cu(1) - O(11)	1.882(3)	Cu(2) - O(21)	1.884(3)
Cu(1) - O(31)	1.938(3)	Cu(2) - O(31)	1.916(3)
Cu(1) - O(41)	1.938(3)	Cu(2) - O(42)	1.941(3)
Cu(1) - N(11)	1.907(4)	Cu(2) - N(21)	1.903(4)
O(11) - C(12)	1.281(6)	O(21) - C(22)	1.285(5)
O(41) - C(41)	1.244(5)	O(42) - C(41)	1.248(5)
N(11) - C(14)	1.303(5)	N(21) - C(24)	1.302(6)
N(11) - C(31)	1.461(6)	N(21) - C(33)	1.461(6)
C(11) - C(12)	1.523(7)	C(21) - C(22)	1.523(7)
C(12) - C(13)	1.361(7)	C(22) - C(23)	1.370(6)
C(13) - C(14)	1.422(7)	C(23) - C(24)	1.409(6)
C(14) - C(15)	1.509(7)	C(24) - C(25)	1.504(6)
C(31) - C(32)	1.515(6)	C(32) - C(33)	1.507(6)
Cu(1) - Cu(2)	3.225(2)		
O(31) - C(32)	1.428(5)		
C(41) - C(42)	1.507(6)		
ATOMS	ANGLE	ATOMS	ANGLE
O(11)-Cu(1)-O(41)	88.6(1)	O(21)-Cu(2)-O(42)	88.3(1)
O(31)-Cu(1)-O(41)	92.0(1)	O(31)-Cu(2)-O(42)	91.8(1)
O(11)-Cu(1)-O(31)	170.0(1)	O(21)-Cu(2)-O(31)	173.1(1)
O(11)-Cu(1)-N(11)	94.6(1)	O(21)-Cu(2)-N(21)	95.2(1)
O(31)-Cu(1)-N(11)	86.2(1)	O(31)-Cu(2)-N(21)	86.2(1)
O(41)-Cu(1)-N(11)	171.5(1)	O(42)-Cu(2)-N(21)	167.3(1)
Cu(1)-O(31)-C(32)	111.6(2)	Cu(2)-O(31)-C(32)	110.2(2)
Cu(1)-O(11)-C(12)	124.9(3)	Cu(2)-O(21)-C(22)	124.5(3)
Cu(1)-O(41)-C(41)	129.1(3)	Cu(2)-O(42)-C(41)	131.5(3)
Cu(1)-N(11)-C(31)	111.8(3)	Cu(2)-N(21)-C(33)	111.3(3)
Cu(1)-N(11)-C(14)	126.8(3)	Cu(2)-N(21)-C(24)	126.1(3)
C(31)-N(11)-C(14)	121.3(4)	C(33)-N(21)-C(24)	122.5(3)
O(11)-C(12)-C(11)	113.6(4)	O(21)-C(22)-C(21)	114.1(4)
O(31)-C(32)-C(31)	109.4(3)	O(31)-C(32)-C(33)	109.3(3)
O(41)-C(41)-C(42)	117.1(4)	O(42)-C(41)-C(42)	116.3(4)
N(11)-C(14)-C(13)	121.1(4)	N(21)-C(24)-C(23)	121.9(4)
N(11)-C(14)-C(15)	120.7(4)	N(21)-C(24)-C(25)	121.2(4)

Table 12. (Continued).

ATOMS	ANGLE	ATOMS	ANGLE
C (11)-C (12)-C (13)	120.1 (4)	C (21)-C (22)-C (23)	120.0 (4)
C (12)-C (13)-C (14)	126.0 (4)	C (22)-C (23)-C (24)	126.3 (4)
C (13)-C (14)-C (15)	118.1 (4)	C (23)-C (24)-C (25)	116.9 (4)
Cu (1)-O (31)-Cu (2)	114.6 (1)		
C (31)-C (32)-C (33)	112.3 (4)		
O (41)-C (41)-O (42)	126.6 (4)		

Table 13. Least Squares Plane Analyses for the complex
 $\text{Cu}_2(\text{Dapac})(\text{OAc})$.^{a,b}

ATOM	DEVIATION (\AA)	ATOM	DEVIATION (\AA)
(a) Equation of the plane involving O(11), O(31), O(41) and N(11):			
$-0.3674x - 0.1036y + 0.9242z = -2.5267$			
O(11)	-0.825	N(11)	0.224
O(31)	0.865	Cu(1)	0.160
O(41)	0.378		
(b) Equation of the plane involving O(21), O(31), O(42) and N(21):			
$-0.1419x + 0.9575y + 0.2513z = 1.9864$			
O(21)	0.146	N(21)	-0.196
O(31)	0.150	Cu(2)	0.336
O(42)	-0.153		

^a Direction cosines of the plane refer to the orthogonal axis system a, b, c^* .

^b All atoms weighted at unity.

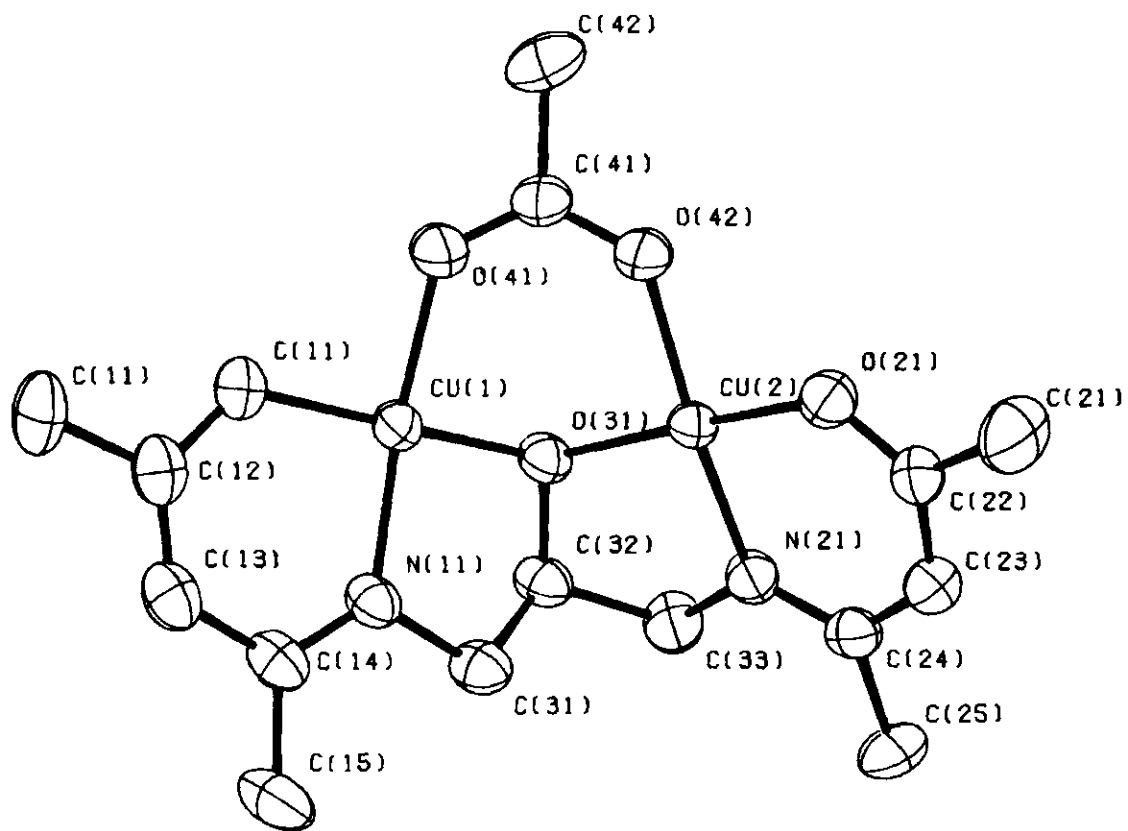


Figure 18. View of the Bent Dinuclear Complex $\text{Cu}_2(\text{Dapac})(\text{OAc})$ with Numbering Scheme Shown.

The one copper(II) atom in the asymmetric unit was easily located from the Patterson synthesis. The remaining non-hydrogen atoms were located from successive difference Fourier calculations. All hydrogen atoms were found geometrically (C - H dist = .95) and their positional parameters were refined, setting their temperature factors constant at 5.0.

The asymmetric unit contains only half of a dinuclear moiety; the remaining part is generated by the symmetry transformation (two-fold axis): $-x, y, 1/2 - z$. The nearest neighbor molecule is generated by inversion.

Tables G and Q contain the structure factors and atomic parameters, respectively. Values of bond distances and angles for this complex, listed in Table 17 and 18, respectively, are compared to the values for the other complexes in this series.

The binuclear complexes (Figure 19) strongly interact with one another along the crystallographic c-axis to form one-dimensional chains (Figure 20). The dinuclear molecule is best described as containing two four-coordinate copper(II) atoms bridged by both the isopropoxide oxygen and the oxygens (three atom bridge) of an acetate group. The coordination sphere of each copper(II) is completed by the phenoxide oxygens and the imine nitrogens of the

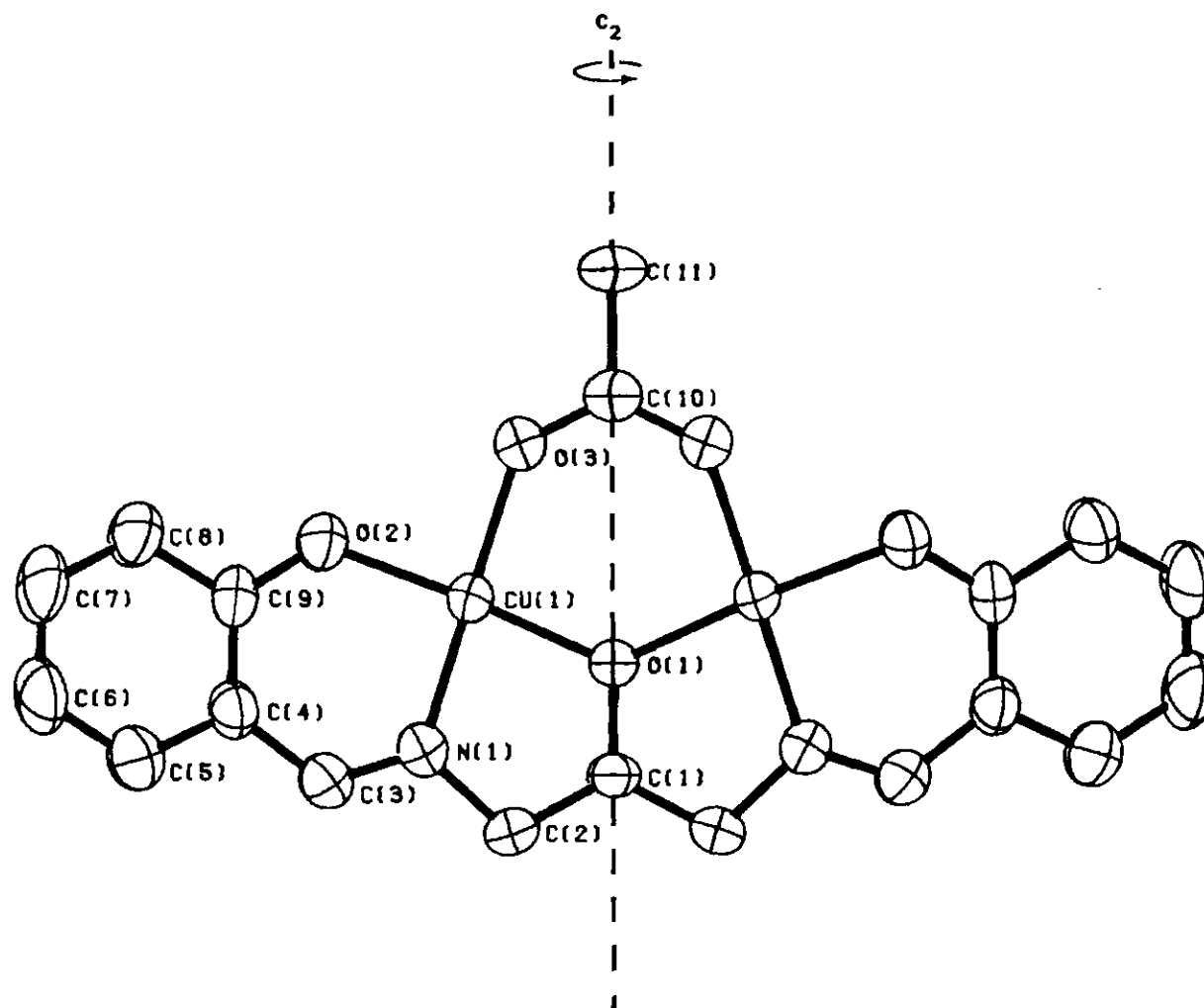


Figure 19. View of the Molecule $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$ Omitting the Two Acetonitrile Molecules of Solvation. The Dashed Line Indicates the Two-Fold Symmetry Axis Imposed by the Space Group $\text{C}2/\text{c}$.

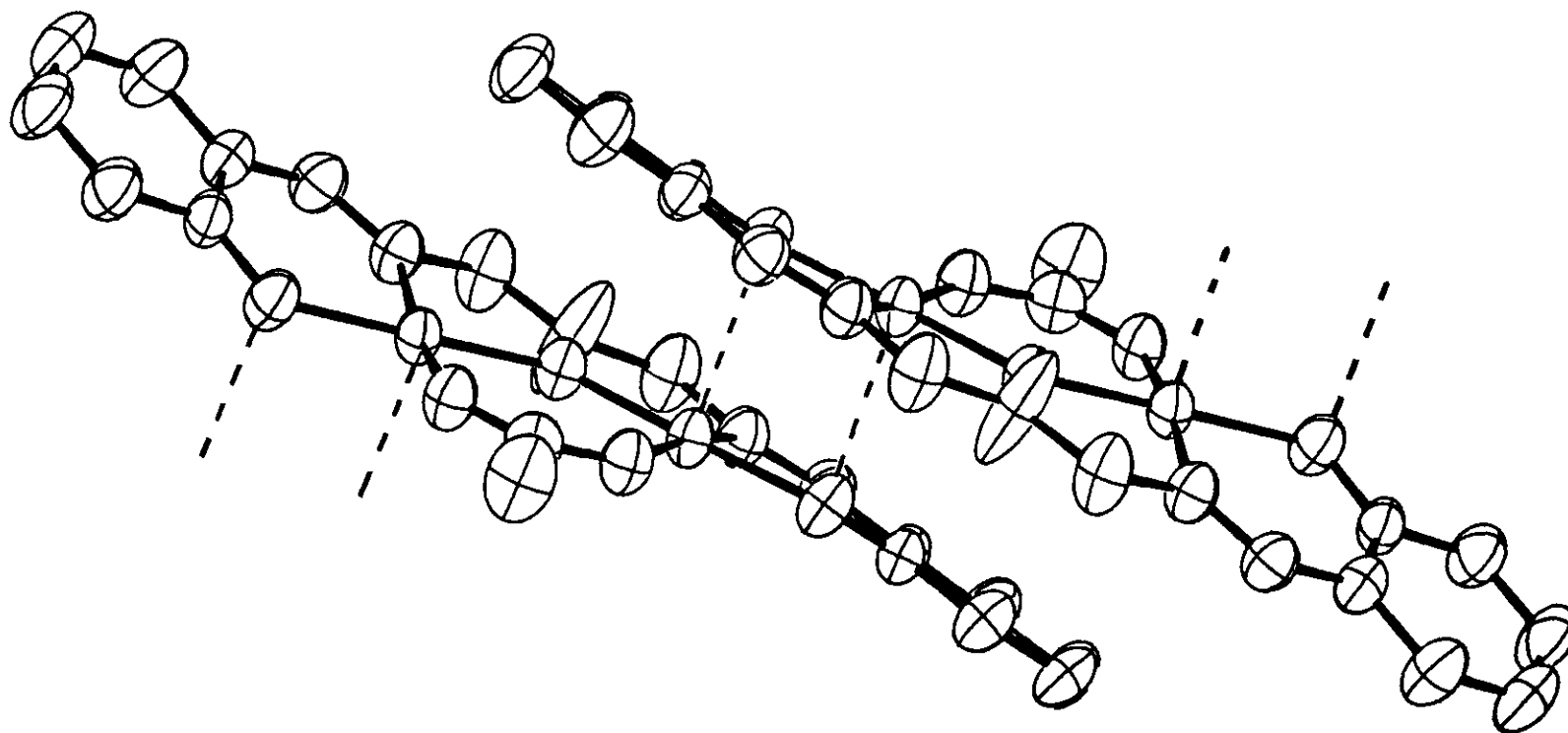
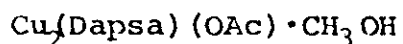


Figure 20. A View of the Intermolecular Infinite Chain Interactions in the Crystal Structure of $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$. Acetonitrile Molecules of Solvation Omitted for Clarity.

binucleating ligand Dapsa. Four membered rings are formed intermolecularly which propagate the infinite chain along the c-axis. These four membered rings consist of two copper(II) atoms bridged by the phenoxide oxygens of Dapsa. The intramolecular Cu(1) - Cu(1') distance (3.463 \AA) is greater than the intermolecular Cu(1) - Cu(1'') distance (3.235 \AA).

The least squares plane analyses (Table 14) for the copper(II) coordination sphere shows little deviation from square planar geometry. The least squares plane analysis for the entire molecule emphasizes just how planar the molecule really is. The largest deviation is found for the atom O(2) (0.623 \AA).

The results of the magnetic study are listed in the second grouping of Table 19, along with the susceptibilities of the other compounds in this series. Since the complex decomposes to the non-solvated species in vacuum, the molar magnetic susceptibilities recorded were calculated using the non-solvated formulation of the complex.



The two copper (II) atoms in the asymmetric unit were easily located from a Patterson synthesis. The remaining atoms were found in successive difference fourier

Table 14. Least Squares Plane Analyses for the Complex
 $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$.^{a,b}

ATOM	DEVIATION (Å)	ATOM	DEVIATION (Å)
(a) Equation of the plane involving O(1), O(2), O(3) and N(1):			
$0.8431x - 0.0788y + 0.5320z = 1.3778$			
O(1)	-0.082	N(1)	0.080
O(2)	-0.090	Cu(1)	-0.073
O(3)	0.073		
(b) Equation of the plane involving the set atoms in a dimer: ^c			
$0.7700x + 0.0104y + 0.6379z = 1.7539$			
Cu(1)	-0.318	Cu(1')	0.234
O(1)	-0.034	C(1)	-0.020
O(2)	-0.623	O(2')	0.525
O(3)	-0.256	O(3')	0.134
N(1)	-0.081	N(1')	0.035
C(2)	-0.040	C(2')	0.014
C(3)	0.084	C(3')	-0.123
C(4)	0.029	C(4')	-0.085
C(5)	0.342	C(5')	-0.386
C(6)	0.295	C(6')	-0.355
C(7)	-0.076	C(7')	-0.012
C(8)	-0.387	C(8')	0.287
C(9)	-0.326	C(9')	0.242
C(10)	-0.067	C(11)	-0.082

^a Direction cosines of the plane refer to the orthogonal axis system a, b, c^* .

^b All atoms weighted at unity.

^c X related to X' by the symmetry transformation: $-x, y, 1/2-z$.

calculations. All hydrogen atoms were located geometrically (C - H dist = 0.95) and their positional parameters refined, setting their temperature factors constant at 5.0.

Tables H and R list the structure factors and atomic parameters, respectively. The bond distances and angles are listed under the second column heading in Table 17 and 18, respectively.

The compound forms discrete, dinuclear units in the solid with the two four-coordinate copper(II) atoms being bridged by the isopropoxide oxygen and the oxygens (three atom bridge) of the acetate group. The coordination sphere of each copper(II) is completed by the phenoxide oxygens and imine nitrogens of the pentadentate ligand (Figure 22, Table 15). The crystal structure of the complex adopts a rather unusual, yet efficient method of packing. This is illustrated in the accompanying ORTEP (Figure 21). The planar complexes are held in this orientation with virtually no intermolecular interaction (closest approach Cu2-C4' = 3.167 Å, Cu-Cu' dist = 3.832 Å).

The magnetic susceptibilities at various temperature are listed in the third set of parameters listed in Table 19.

Cu₂(Dapsa) (OAc)

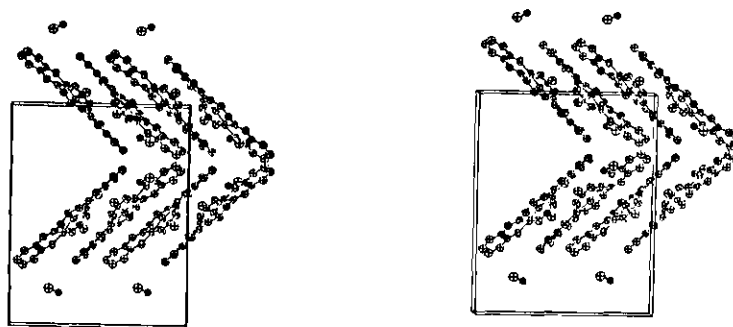


Figure 21. Stereoview of the Unit Cell and Packing Diagram for the Complex $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$.

Only two of the four copper(II) atoms in the asymmetric unit could be located from the rather complicated Patterson synthesis. In the following difference Fourier the remaining two copper(II) atoms were located along with the atoms in the coordination sphere of each metal. The remaining atoms were found from successive difference Fourier calculations.

Tables I and S in the appendix contain the structure factors and atomic parameters, respectively, for the complex. Selected bond distances and angles are listed in the third group of parameters in Tables 17 and 18 respectively. In these tables the equivalence of the analogous portions of the molecule is easily seen.

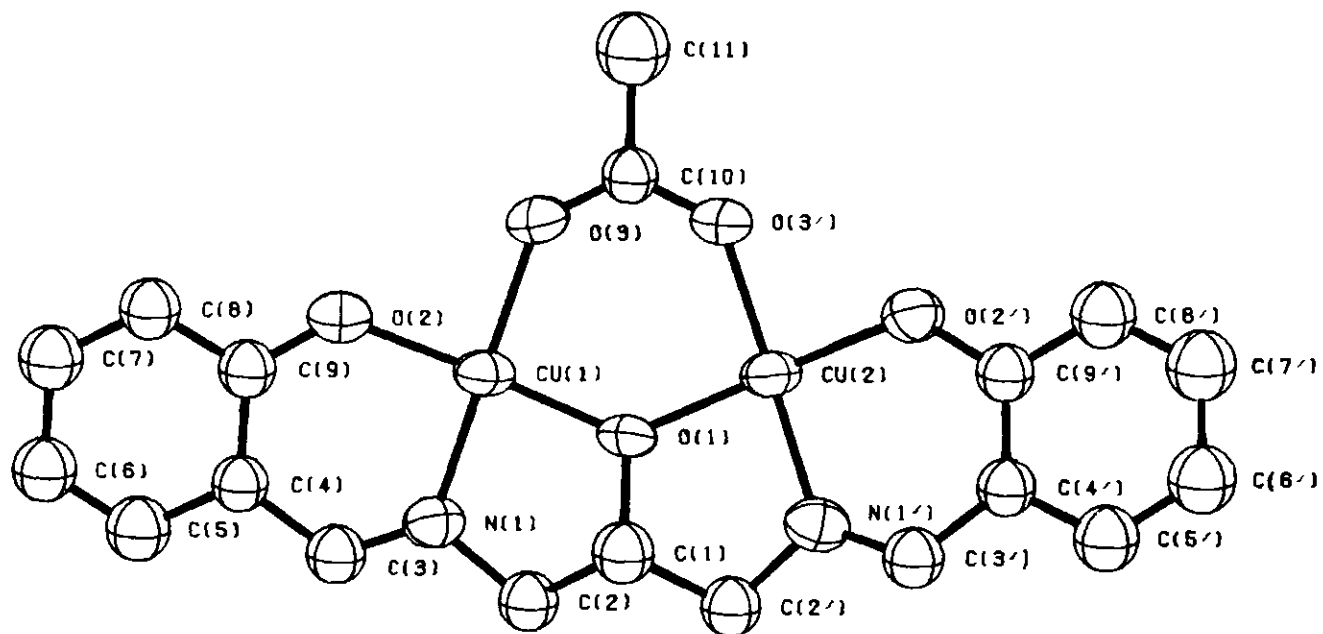


Figure 22. View of the Molecule $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ Omitting the Methanol Molecule of Solvation.

Table 15. Least Squares Plane Analyses for the Complex
 $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$.^{a, b}

ATOM	DEVIATION (Å)	ATOM	DEVIATION (Å)
(a) Equation of the plane involving O(1), O(2), O(3) and N(1):			
$-0.2102x - 0.7454y + 0.6327z = -1.7326$			
O(1)	-0.113	N(1)	0.139
O(2)	-0.112	Cu(1)	0.010
O(3)	0.119		
(b) Equation of the plane involving O(1), O(2'), O(3') and N(1'):			
$-0.3214x - 0.6431y + 0.6950z = -1.5946$			
O(1)	-0.015	N(1')	0.016
O(2')	-0.016	Cu(2)	0.061
O(3')	0.016		
(c) Equation of the plane involving the set of atoms in a dimer:			
$-0.2887x - 0.6505y + 0.7026z = -1.7908$			
Cu(1)	0.043	Cu(2)	0.286
O(1)	0.181	C(1)	-0.104
O(2)	-0.333	O(2')	0.236
O(3)	0.068	O(3')	0.302
N(1)	0.257	N(1')	0.179
C(2)	0.493	C(2')	0.374
C(3)	0.267	C(3')	-0.076
C(4)	0.082	C(4')	-0.153
C(5)	0.186	C(5')	-0.425
C(6)	0.049	C(6')	-0.507
C(7)	-0.292	C(7')	-0.163
C(8)	-0.417	C(8')	0.086
C(9)	-0.236	C(9')	0.070
C(10)	0.193	C(11)	0.262

^a Direction cosines of the plane refer to the orthogonal system a, b, c^* .

^b All atoms weighted at unity.

The two independent dinuclear molecules are similar in gross structure. Two four-coordinate copper(II) atoms are bridged by an isopropoxide oxygen of the Dapsa ligand and by the oxygens (three atom bridge) of the acetate group. The remaining coordination sites at each copper(II) are filled by the phenoxide oxygens and the imine nitrogens of the ligand. The two crystallographically independent molecules are illustrated in Figure 23 as they occur in the asymmetric unit.

The least squares plane analyses of the coordination spheres of the metal atoms shows only minor deviations from idealized square planar geometry (Table 16). The overall planarity of the molecule is evident from the results listed in the last two analyses of Table 16.

The magnetic susceptibilities at various temperatures are reported in the fourth set of values listed in Table 19.

Cu(DapsaH) · CH₃CN

The one copper(II) atom in the asymmetric unit was located via a Patterson synthesis. All the coordinating atoms were found on the first difference Fourier calculation, with the remaining atoms being located on successive Fourier electron density maps.

Table 16. Least Squares Plane Analyses for the Complex
 $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.^{a,b}

ATOM	DEVIATION (Å)	ATOM	DEVIATION (Å)
(a) Equation of the plane involving O11, O21, O31 and N11:			
$0.0646x - 0.6018y + 0.7961z = -1.0949$			
O11	-0.058	N11	0.060
O21	-0.104	Cu(1)	0.012
O31	0.134		
(b) Equation of the plane involving O11, O2'1, O3'1 and N1'1:			
$-0.1686x - 0.5949y + 0.7859z = -1.4974$			
O11	-0.163	N1'1	0.121
O2'1	-0.111	Cu(2)	0.017
O3'1	0.222		
(c) Equation of the plane involving O12, O22, O32 and N12:			
$-0.0414x + 0.9858y + 0.1629z = -1.2889$			
O12	-0.011	N12	0.027
O22	-0.144	Cu(3)	0.003
O32	0.167		
(d) Equation of the plane involving O12, O2'2, O3'2 and N1'2:			
$-0.0238x + 0.9663y + 0.2565z = -0.6911$			
O12	-0.021	N1'2	0.018
O2'2	-0.015	Cu(4)	0.027
O3'2	0.020		

^a Direction cosines of the plane refer to the orthogonal axis system a, b, c^* .

^b All atoms weighted at unity.

Table 16. (Continued).

ATOM	DEVIATION (Å) ^a	ATOM	DEVIATION (Å) ^a
(e) Equation of the plane involving the set of atoms in the #1 dimer:			
$-0.0274x - 0.7134y + 0.7000z = -2.3959$			
Cu(1)	0.483	Cu(2)	0.505
O11	0.457	C11	-0.100
O21	0.316	O2'1	0.240
O31	0.926	O3'1	1.058
N11	0.209	N1'1	0.256
C21	0.362	C2'1	0.389
C31	-0.148	C3'1	0.004
C41	-0.294	C4'1	-0.093
C51	-0.699	C5'1	-0.344
C61	-0.864	C6'1	-0.454
C71	-0.643	C7'1	-0.312
C81	-0.221	C8'1	-0.061
C91	-0.072	C9'1	0.048
C101	1.269	C111	1.931
(f) Equation of the plane involving the set of atoms in the #2 dimer:			
$-0.0327x + 0.9810y + 0.1914z = -1.0525$			
Cu(3)	-0.042	Cu(4)	0.066
O12	-0.048	C12	-0.251
O22	-0.195	O2'2	0.085
O32	0.064	O3'2	0.174
N12	0.040	N1'2	-0.058
C22	0.098	C2'2	-0.031
C32	0.089	C3'2	-0.098
C42	0.025	C4'2	-0.022
C52	0.177	C5'2	-0.038
C62	0.073	C6'2	0.032
C72	-0.146	C7'2	0.132
C82	-0.257	C8'2	0.185
C92	-0.136	C9'2	0.085
C102	0.194	C112	0.456

^a Direction cosines of the plane refer to the orthogogonal axis system a,b,c*.

^b All atoms weighted at unity.

Table 17. Comparison of Selected Analogous Interatomic Bond Distances (Å) for $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$, $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ and $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$

	ATOMS	DIST.
1	Cu(1) - O(1)	1.902(2)
2	Cu(1) - O(2)	1.909(3)
3	Cu(1) - O(3)	1.931(4)
4	Cu(1) - N(1)	1.926(4)
5	O(2) - C(9)	1.318(6)
6	O(3) - C(10)	1.253(5)
7	N(1) - C(2)	1.464(7)
8	N(1) - C(3)	1.276(6)
9	C(1) - C(2)	1.417(8)
10	C(3) - C(4)	1.412(7)
11	C(4) - C(5)	1.407(7)
12	C(5) - C(6)	1.367(9)
13	C(6) - C(7)	1.375(9)
14	C(7) - C(8)	1.364(8)
15	C(8) - C(9)	1.417(7)
16	C(4) - C(9)	1.395(7)
17	O(1) - C(1)	1.338(9)
18	C(10) - C(11)	1.51(1)
19	Cu(1) - Cu(1')	3.463(2)

	ATOMS	DIST.		ATOMS	DIST.
	Cu(1) - O(1)	1.829(4)		Cu(2) - O(1)	1.904(4)
	Cu(1) - O(2)	1.885(5)		Cu(2) - O(2')	1.891(4)
	Cu(1) - O(3)	1.940(4)		Cu(2) - O(3')	1.925(4)
	Cu(1) - N(1)	1.923(5)		Cu(2) - N(1')	1.912(5)
	O(2) - C(9)	1.301(7)		O(2') - C(9')	1.317(7)
	O(3) - C(10)	1.227(7)		O(3') - C(10)	1.236(7)
	N(1) - C(2)	1.492(8)		N(1') - C(2')	1.459(8)
	N(1) - C(3)	1.253(7)		N(1') - C(3')	1.278(8)
	C(1) - C(2)	1.50(1)		C(1) - C(2')	1.48(1)
	C(3) - C(4)	1.427(8)		C(3') - C(4')	1.418(8)
	C(4) - C(5)	1.404(8)		C(4') - C(5')	1.416(9)
	C(5) - C(6)	1.336(9)		C(5') - C(6')	1.35(1)
	C(6) - C(7)	1.376(9)		C(6') - C(7')	1.40(1)
	C(7) - C(8)	1.359(9)		C(7') - C(8')	1.380(9)
	C(8) - C(9)	1.400(9)		C(8') - C(9')	1.382(9)
	C(4) - C(9)	1.419(9)		C(4') - C(9')	1.400(8)
	O(1) - C(1)	1.416(7)			
	C(10) - C(11)	1.52(1)			
	Cu(1) - Cu(2)	3.482(2)			

$\text{Cu}_2(\text{Dapsa})(\text{OAc})$

	ATOMS	DIST.
1	Cu(1) - O(11)	1.903(6)
2	Cu(1) - O(21)	1.883(6)
3	Cu(1) - O(31)	1.916(6)
4	Cu(1) - N(11)	1.901(7)
5	O(21) - C(91)	1.32(1)
6	O(31) - C(101)	1.23(1)
7	N(11) - C(21)	1.47(1)
8	N(11) - C(31)	1.29(1)
9	C(11) - C(21)	1.54(1)
10	C(31) - C(41)	1.43(1)
11	C(41) - C(51)	1.43(1)
12	C(51) - C(61)	1.36(1)
13	C(61) - C(71)	1.41(1)
14	C(71) - C(81)	1.41(1)
15	C(81) - C(91)	1.38(1)
16	C(41) - C(91)	1.39(1)
17	O(11) - C(11)	1.52(1)
18	C(101) - C(111)	1.41(1)
19	Cu(1) - Cu(2)	3.470(2)

	ATOMS	DIST.		ATOMS	DIST.
	Cu(2) - O(11)	1.902(6)		Cu(3) - O(12)	1.902(6)
	Cu(2) - O(2'1)	1.868(6)		Cu(3) - O(22)	1.868(5)
	Cu(2) - O(3'1)	1.911(6)		Cu(3) - O(32)	1.920(6)
	Cu(2) - N(1'1)	1.923(7)		Cu(3) - N(12)	1.910(7)
	O(2'1) - C(9'1)	1.33(1)		O(22) - C(92)	1.32(1)
	O(3'1) - C(101)	1.25(1)		O(32) - C(102)	1.25(1)
	N(1'1) - C(2'1)	1.48(1)		N(12) - C(22)	1.47(1)
	N(1'1) - C(3'1)	1.28(1)		N(12) - C(32)	1.28(1)
	C(1'1) - C(2'1)	1.53(1)		C(12) - C(22)	1.46(1)
	C(3'1) - C(4'1)	1.45(1)		C(32) - C(42)	1.45(1)
	C(4'1) - C(5'1)	1.44(1)		C(42) - C(52)	1.45(1)
	C(5'1) - C(6'1)	1.38(1)		C(52) - C(62)	1.37(1)
	C(6'1) - C(7'1)	1.35(1)		C(62) - C(72)	1.38(1)
	C(7'1) - C(8'1)	1.39(1)		C(72) - C(82)	1.40(1)
	C(8'1) - C(9'1)	1.42(1)		C(82) - C(92)	1.42(1)
	C(4'1) - C(9'1)	1.39(1)		C(42) - C(92)	1.38(1)
				O(12) - C(12)	1.37(1)
				C(102) - C(112)	1.49(1)
				Cu(3) - Cu(4)	3.482(2)

Table 18. Comparison of Selected Analogous Interatomic Bonding Angles (deg) for $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$, $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$, and $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$			$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$			
	ATOMS	ANGLE	ATOMS	ANGLE	ATOMS	ANGLE
1	O1-Cu1-O3	96.0(2)	O1-Cu1-O3	94.2(2)	O1-Cu2-O3'	94.5(2)
2	O2-Cu1-O3	88.0(2)	O2-Cu1-O3	88.6(2)	O2'-Cu2-O3'	86.8(2)
3	O1-Cu1-O2	176.0(2)	O1-Cu1-O2	172.2(2)	O1-Cu2-O2'	175.1(2)
4	O1-Cu1-N1	83.5(2)	O1-Cu1-N1	85.4(2)	O1-Cu2-N1'	84.3(2)
5	O2-Cu1-N1	92.7(2)	O2-Cu1-N1	92.7(2)	O2'-Cu2-N1'	94.1(2)
6	O3-Cu1-N1	171.1(2)	O3-Cu1-N1	172.9(2)	O3'-Cu2-N1'	177.1(2)
7	Cu1-O1-C1	114.5(1)	Cu1-O1-C1	111.9(4)	Cu2-O1-C1	113.8(4)
8	Cu1-O2-C9	125.4(3)	Cu1-O2-C9	128.0(4)	Cu2-O2'-C9'	126.7(4)
9	Cu1-O3-C10	135.2(4)	Cu1-O3-C10	135.0(4)	Cu2-O3'-C10	134.6(5)
10	Cu1-N1-C2	113.3(3)	Cu1-N1-C2	111.4(4)	Cu2-N1'-C2'	113.0(4)
11	Cu1-N1-C3	126.2(4)	Cu1-N1-C3	127.1(4)	Cu2-N1'-C3'	125.6(4)
12	C2-N1-C3	120.4(5)	C2-N1-C3	121.5(5)	C2'-N1'-C3'	121.3(5)
13	O1-C1-C2	118.0(4)	O1-C1-C2	108.7(5)	O1-C1-C2'	110.5(5)
14	C1-C2-N1	109.7(6)	C1-C2-N1	107.4(5)	C1-C2'-N1'	107.6(5)
15	N1-C3-C4	125.3(5)	N1-C3-C4	125.3(6)	N1'-C3'-C4'	124.9(6)
16	C3-C4-C5	117.2(5)	C3-C4-C5	119.2(6)	C3'-C4'-C5'	117.2(6)
17	C5-C4-C9	119.5(5)	C5-C4-C9	118.0(6)	C5'-C4'-C9'	118.3(6)
18	C3-C4-C9	123.2(4)	C3-C4-C9	122.8(6)	C3'-C4'-C9'	124.5(6)
19	C4-C5-C6	121.6(6)	C4-C5-C6	122.9(6)	C4'-C5'-C6'	122.6(7)
20	C5-C6-C7	118.7(6)	C5-C6-C7	119.2(6)	C5'-C6'-C7'	118.8(7)
21	C6-C7-C8	118.7(6)	C6-C7-C8	120.6(6)	C6'-C7'-C8'	119.7(7)
22	C7-C8-C9	120.7(6)	C7-C8-C9	121.9(6)	C7'-C8'-C9'	122.2(7)
23	C4-C9-C8	117.7(5)	C4-C9-C8	117.3(6)	C4'-C9'-C8'	118.4(6)
24	O2-C9-C4	124.7(4)	O2-C9-C4	123.4(5)	O2'-C9'-C4'	123.2(6)
25	O2-C9-C8	117.6(5)	O2-C9-C8	119.3(6)	O2'-C9'-C8'	118.5(7)
26	O3-C10-C11	116.7(3)	O3-C10-C11	116.5(6)	O3'-C10-C11	114.9(6)
27	Cu1-O1-Cu1'	131.1(2)	Cu1-O1-Cu2	133.0(2)		
28	C2-C1-C2'	113.6	C2-C1-C2'	113.3(5)		
29	O3-C10-O3'	126.6(7)	O3-C10-O3'	128.5(6)		

Table 18. (Continued).

Cu ₂ (Dapsa) (OAc)								
	ATOMS	ANGLE	ATOMS	ANGLE	ATOMS	ANGLE	ATOMS	ANGLE
1	O11-Cu1-O31	94.5(3)	O11-Cu2-O3'1	94.2(3)	O12-Cu3-O32	95.1(3)	O12-Cu4-O3'2	94.3(2)
2	O21-Cu1-O31	88.4(3)	O2'1-Cu2-O3'1	88.9(3)	O22-Cu3-O32	87.4(3)	O2'2-Cu4-O3'2	87.3(3)
3	O11-Cu1-O21	173.8(3)	O11-Cu2-O2'1	170.4(3)	O12-Cu3-O22	174.6(3)	O12-Cu4-O2'2	176.9(3)
4	O11-Cu1-N11	84.7(3)	O11-Cu2-N1'1	84.6(3)	O12-Cu3-N12	84.1(3)	O12-Cu4-N1'2	84.3(3)
5	O21-Cu1-N11	93.0(3)	O2'1-Cu2-N1'1	93.9(3)	O22-Cu3-N12	93.8(3)	O2'2-Cu4-N1'2	94.1(3)
6	O31-Cu1-N11	174.8(3)	O3'1-Cu2-N1'1	170.5(3)	O32-Cu3-N12	174.4(3)	O3'2-Cu4-N1'2	178.5(3)
7	Cu1-O11-C11	112.7(5)	Cu2-O11-C11	112.4(5)	Cu3-O12-C12	113.9(5)	Cu4-O12-C12	113.9(5)
8	Cu1-O21-C91	127.3(6)	Cu2-O2'1-C9'1	126.9(5)	Cu3-O22-C92	127.5(5)	Cu4-O2'2-C9'2	125.3(6)
9	Cu1-O31-C101	134.6(6)	Cu2-O3'1-C101	135.3(6)	Cu3-O32-C102	135.8(6)	Cu4-O3'2-C102	137.6(6)
10	Cu1-N11-C21	112.9(5)	Cu2-N1'1-C2'1	112.5(6)	Cu3-N12-C22	114.1(6)	Cu4-N1'2-C2'2	114.4(6)
11	Cu1-N11-C31	128.0(6)	Cu2-N1'1-C3'1	127.8(6)	Cu3-N12-C32	127.3(6)	Cu4-N1'2-C3'2	128.8(6)
12	C21-N11-C31	119.1(8)	C2'1-N1'1-C3'1	119.6(7)	C22-N12-C32	118.5(8)	C2'2-N1'2-C3'2	116.7(7)
13	O11-C11-C21	107.4(1)	O11-C11-C2'1	108.3(7)	O12-C12-C22	114.8(9)	O12-C12-C2'2	116.7(9)
14	C11-C21-N11	105.2(7)	C11-C2'1-N1'1	104.8(7)	C12-C22-N12	108.2(8)	C12-C'2'-N1'2	107.9(9)
15	N11-C31-C41	122.9(9)	N1'1-C3'1-C4'1	122.2(8)	N12-C32-C42	122.7(8)	N1'2-C3'2-C4'2	122.4(8)
16	C31-C41-C51	115.4(8)	C3'1-C4'1-C5'1	115.0(8)	C32-C42-C52	114.5(8)	C3'2-C4'2-C5'2	115.6(9)
17	C51-C41-C91	120.2(8)	C5'1-C4'1-C9'1	120.1(8)	C52-C42-C92	120.9(5)	C5'2-C4'2-C9'2	120.9(9)
18	C31-C41-C91	124.4(8)	C3'1-C4'1-C9'1	124.9(8)	C32-C42-C92	124.6(8)	C3'2-C4'2-C9'2	123.5(8)
19	C41-C51-C61	120.1(9)	C4'1-C5'1-C6'1	119.9(1)	C42-C52-C62	117.9(9)	C4'2-C5'2-C6'2	118.7(9)
20	C51-C61-C71	120(1)	C5'1-C6'1-C7'1	120(1)	C52-C62-C72	122(1)	C5'2-C6'2-C7'2	121(1)
21	C61-C71-C81	120.2(9)	C6'1-C7'1-C8'1	124(1)	C62-C72-C82	121(1)	C6'2-C7'2-C8'2	122(1)
22	C71-C81-C91	119.9(9)	C7'1-C8'1-C9'1	117.4(8)	C72-C82-C92	118.7(8)	C7'2-C8'2-C9'2	120(1)
23	C41-C91-C81	119.7(8)	C4'1-C9'1-C8'1	119.5(8)	C42-C92-C82	119.5(8)	C4'2-C9'2-C8'2	118.3(9)
24	O21-C91-C41	123.8(8)	O2'1-C9'1-C4'1	124.1(8)	O22-C92-C42	123.8(7)	O2'2-C9'2-C4'2	125.7(8)
25	O21-C91-C81	116.5(8)	O2'1-C9'1-C8'1	116.4(8)	O22-C92-C82	116.8(8)	O2'2-C9'2-C8'2	115.9(8)
26	O31-C101-C111	117.4(9)	O3'1-C101-C111	116.2(9)	O32-C102-C112	117.3(8)	O3'2-C102-C112	117.8(8)
27	Cu1-O11-Cu2	131.6(3)			Cu3-O12-Cu4	132.1(3)		
28	C21-C11-C2'1	111.8(7)			C22-C12-C2'2	118.8(9)		
29	O31-C101-O3'1	126.2(9)			O32-C102-O3'2	124.9(8)		

Table 19. Diamagnetic Corrections (χ_{dia}), Molar Magnetic Susceptibilities ($\chi_{\text{M}}^{\text{corr}}$) and Effective Magnetic Moments (μ_{eff}) for the Complexes $\text{Cu}_2(\text{Dapac})(\text{OAc})$, $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$, $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ and $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.

T (°K)	$\chi_{\text{M}}^{\text{corr}} \times 10^6 \text{ cgs}$	μ_{eff} (BM)	$\chi_{\text{M}}^{\text{corr}} \times 10^6 \text{ cgs}$	μ_{eff} (BM)
$\text{Cu}_2(\text{Dapac})(\text{OAc})$			$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot [2\text{CH}_3\text{CN}]$	
	$\chi_{\text{dia}} = -0.000093$		$\chi_{\text{dia}} = -0.000104$	
298	1519	1.90	1310	1.76
278	1632	1.91	1346	1.73
258	1769	1.91	1438	1.72
238	1922	1.91	1512	1.70
218	2101	1.92	1608	1.68
198	2325	1.92	1715	1.65
178	2601	1.93	1842	1.62
158	2948	1.93	1923	1.56
138	3440	1.95	2065	1.51
118	4075	1.96	2181	1.44
98	4922	1.97	2297	1.34
$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$			$\text{Cu}_2(\text{Dapsa})(\text{OAc})$	
	$\chi_{\text{dia}} = -0.000115$		$\chi_{\text{dia}} = -0.000104$	
298	1226	1.71	1201	1.68
278	1273	1.68	1237	1.66
258	1343	1.67	1301	1.64
238	1395	1.63	1355	1.61
218	1461	1.60	1423	1.58
198	1511	1.55	1483	1.53
178	1540	1.48	1536	1.48
158	1547	1.40	1568	1.41
138	1486	1.28	1575	1.32
118	1352	1.13	1517	1.20
98	1101	0.93	1391	1.05

Tables J and T contain the structure factors and atomic parameters, respectively, for this complex. Selected bond distances and angles for this complex are listed in Table 20.

The compound crystallizes with four discrete, monomeric units in the unit cell. The four coordinate copper(II) atom is chelated, in a cisoid fashion, by two imine nitrogens and two phenoxide oxygens of the Dapsa ligand. The remaining protonated isopropyl oxygen is uncoordinated, but is weakly hydrogen-bonded (2.70 \AA O-O dist.) to the phenoxide oxygen of an adjacent molecule. The structure and labeling system are presented in Figure 24.

Several interesting structural aspects arise in this complex due to the strain imposed by the saturated diaminopropane moiety of the ligand. The six membered ring formed as a result of the coordination of the two imine nitrogens to the copper(II), assumes a severely twisted conformation. four of the atoms contained in this ring (Cu1 N11 N21 and C1) all lie in a plane whereas C11 is well below (0.674 \AA) and C21 is well above (-0.745 \AA) the plane (Figure 25). The idealized square planar geometry about the central metal atom is distorted toward tetrahedral geometry (Table 21).

The magnetic susceptibility of this monomer was not experimentally determined. It was assumed to be a magnetically dilute, one unpaired electron system with a moment, independent of temperature, in the range of 1.73 - 1.90 BM.

Table 20. Selected Interatomic Distances (Å) and Angles (deg)
for Cu(DapsaH)·CH₃CN.

ATOMS	n=	1	2
DISTANCES			
Cu-O(n1)		1.913(9)	1.92(1)
Cu-N(n1)		1.92(1)	1.95(1)
O(n1)-C(n8)		1.29(1)	1.32(2)
N(n1)-C(n1)		1.49(2)	1.50(2)
N(n1)-C(n2)		1.28(2)	1.31(2)
C(1)-C(n1)		1.56(2)	1.49(2)
C(n2)-C(n3)		1.46(2)	1.43(2)
C(n3)-C(n4)		1.46(2)	1.48(2)
C(n4)-C(n5)		1.40(2)	1.34(2)
C(n5)-C(n6)		1.40(2)	1.47(2)
C(n6)-C(n7)		1.39(2)	1.40(2)
C(n7)-C(n8)		1.43(2)	1.42(2)
C(n3)-C(n8)		1.40(2)	1.37(2)
C(n)-O(n)		1.46(2)	
NSOLV-C1SLV		1.12(2)	
C1SLV-C2SLV		1.50(3)	

ATOMS	n=	1	2
ANGLES			
Cu-O(n1)-C(n8)		127.5(9)	126.4(9)
Cu-N(n1)-C(n1)		116(1)	114(1)
Cu-N(n1)-C(n2)		129(1)	125(1)
C(n1)-N(n1)-C(n2)		115(1)	121(1)
O(1)-C(1)-C(n1)		103(1)	116(1)
O(n1)-C(n8)-C(n3)		124(1)	123(1)
O(n1)-C(n8)-C(n7)		116(1)	116(2)
N(n1)-C(n2)-C(n3)		122(2)	123(2)
C(1)-C(n1)-N(n1)		113(1)	114(1)
C(n2)-C(n3)-C(n4)		115(2)	113(1)
C(n2)-C(n3)-C(n8)		124(2)	128(2)
C(n4)-C(n3)-C(n8)		120(2)	119(2)
C(n3)-C(n4)-C(n5)		119(2)	119(2)
C(n4)-C(n5)-C(n6)		120(2)	122(2)
C(n5)-C(n6)-C(n7)		123(2)	118(2)
C(n6)-C(n7)-C(n8)		118(2)	120(2)
C(n7)-C(n8)-C(n3)		120(1)	121(2)

Table 20. (Continued).

ATOMS	ANGLE	ATOMS	ANGLE
O(11)-Cu-N(11)	91.9(5)	O(22)-Cu-N(22)	94.2(5)
O(11)-Cu-O(21)	91.8(4)	N(11)-Cu-N(21)	93.0(6)
N(11)-Cu-O(21)	156.0(5)	O(11)-Cu-N(21)	153.6(6)
NSOLV-C1SLV-C2SLV	169.9		

Table 21. Least Squares Plane Analysis for the Monomeric Complex $\text{Cu}(\text{DapsaH}) \cdot \text{CH}_3\text{CN}$.^{a, b}

ATOM	DEVIATION (Å)	ATOM	DEVIATION (Å)
(a) Equation of the plane involving O11, O21, N11 and N21:			
$0.3311x + 0.9405y + 0.0757z = 2.0759$			
O11	-0.434	N21	-0.588
O21	0.286	Cu	-0.071
N11	0.373		
(b) Equation of the plane involving the four atoms Cu, N21, N11 and C1 (six-membered ring):			
$0.6321x + 0.7675y + 0.1068z = 1.5560$			
Cu	0.056	C1	0.039
N11	-0.047	N21	-0.054
C11	0.674	C21	-0.745

^a Direction cosines of the plane refer to the orthogonal axis system a, b, c*.

^b All atoms weighted at unity.

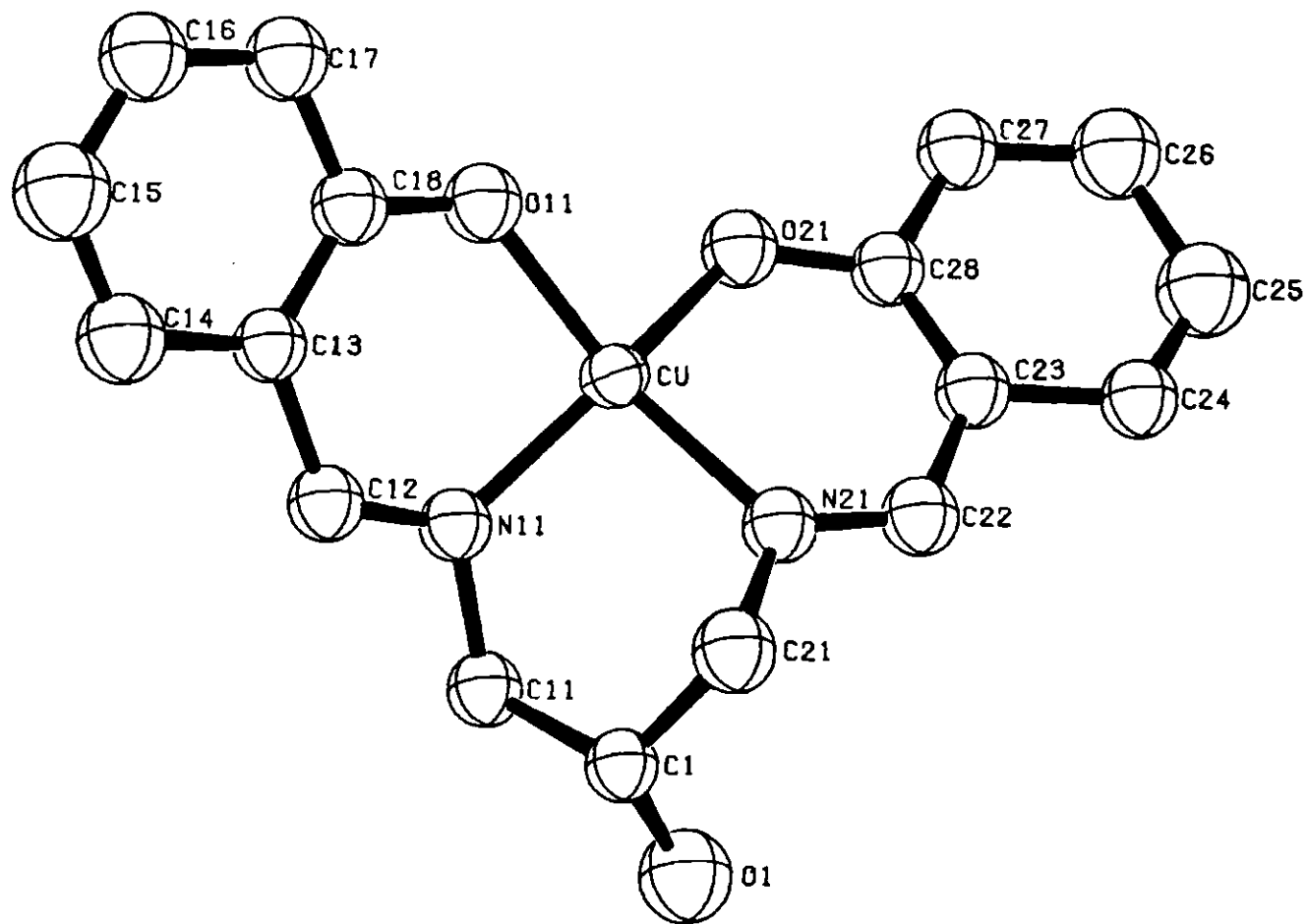


Figure 24. View of the Monomeric Complex $\text{Cu}(\text{DapsaH}) \cdot \text{CH}_3\text{CN}$ with Numbering Scheme. The Acetonitrile Molecule of Solvation has been Omitted for Clarity.

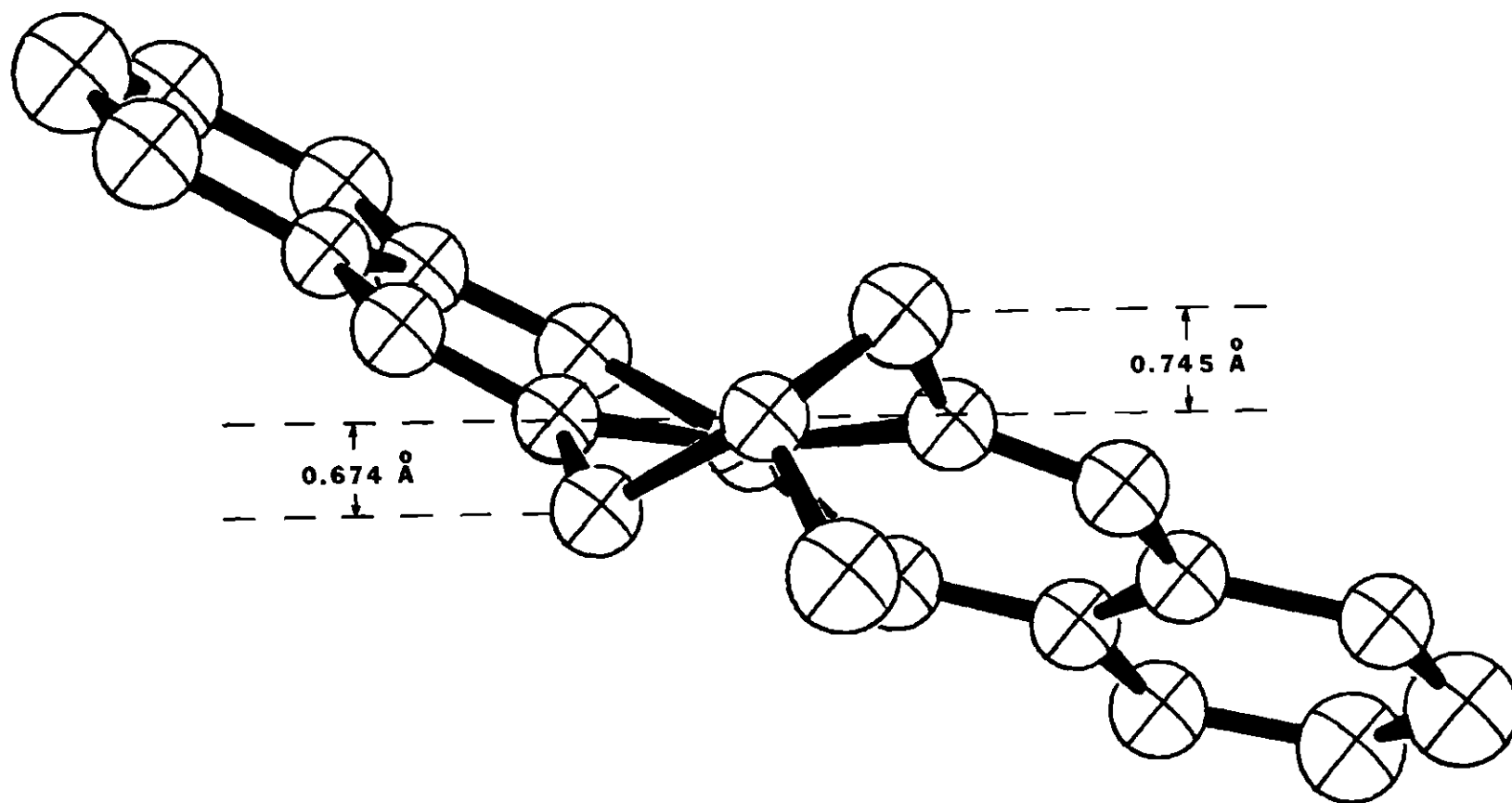


Figure 25. View of $\text{Cu}(\text{DapsaH}) \cdot \text{CH}_3\text{CN}$ Showing Conformation of the Distorted Six-Membered Ring. Distances Specified are the Deviations of C(11) and C(21) from the Plane Defined by Cu, N(11), N(21) and C(1).

CHAPTER III

DISCUSSION OF RESULTS

This chapter will highlight only the structural and magnetic results of comparative interest. Selected bond distances and angles of the complexes studied are summarized in Chapter II along with the detailed description of each molecular and crystal structure.

The advent of automated, variable scan rate X-ray diffractometers made possible the structural determination of several complexes which were unstable to air. This can be attributed to both the speed with which a full data set can now be collected and also the elimination of the need to perform preliminary camera work (i.e. no need for crystal to be aligned along an axis).

Results

Cubane-like Complexes

Cubane-like structures have been found for both the alpha- and beta-forms of Cu(EIA) (Figure 26). The

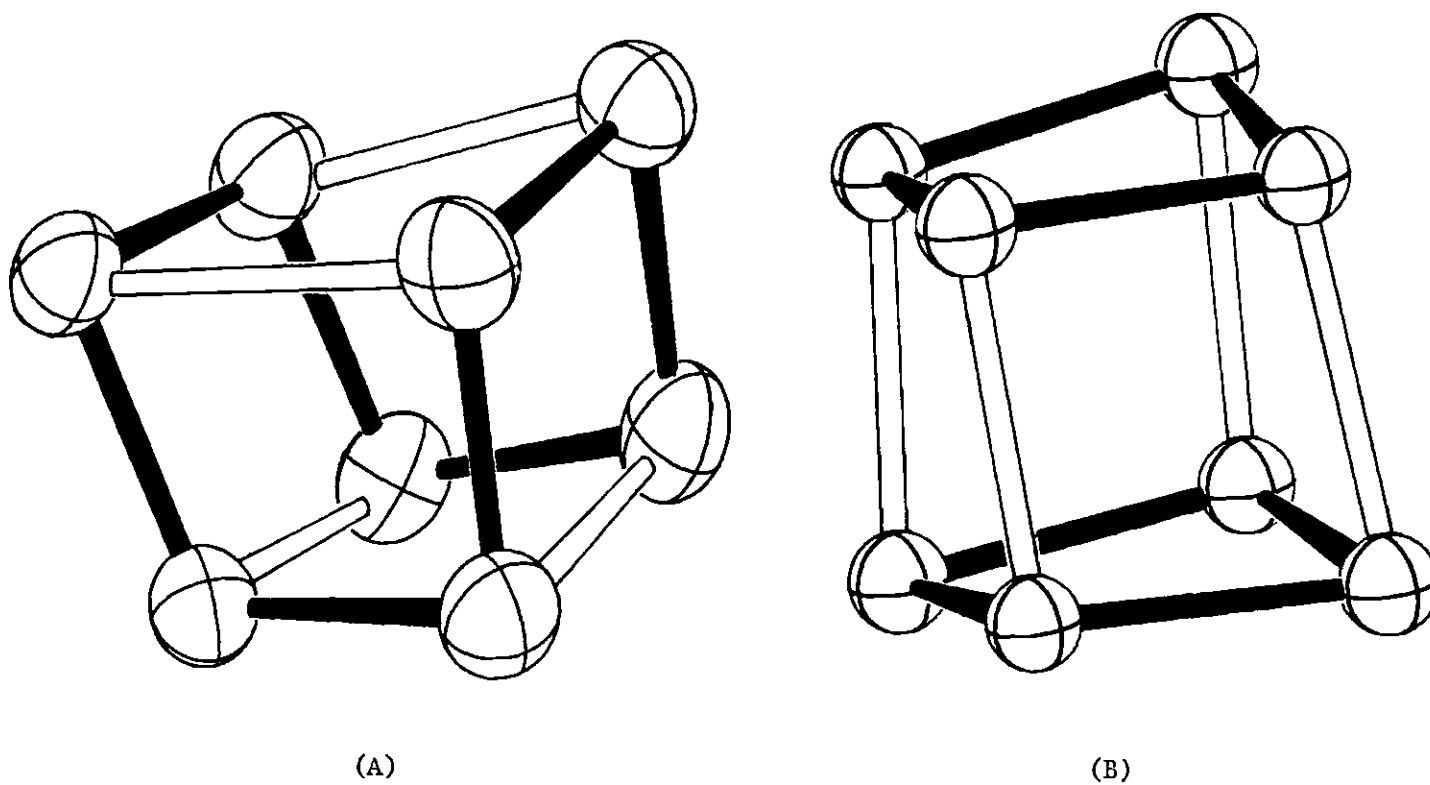


Figure 26. Comparative Views of the Cubane Units. (A) The Tub Conformation Which β -[Cu(EIA)]₄ Adopts and (B) the Associated Dimer Form Which α -[Cu(EIA)]₄ Assumes.

alpha- and beta-forms differ in the coordination to copper, the relative orientation of ligands, and in the relative positions of short and long Cu-O "cube" edges. The alpha-form, structurally characterized in 1970 (9), can be thought of as two associated dimers with each copper assuming a trigonal bipyramidal geometry (Figure 26B). The beta-form (presented herein) is best described as a folded 8-membered ring in a tub-like conformation (similar to cyclooctatetraene); each copper is square pyramidal (Figure 26A).

Shortly after the solvated beta-form had been structurally characterized in our laboratory (2-butanol solvate), Haase and coworkers (34) reported a dibenzene solvate with the same tub-like geometry. Helm had also prepared a homologous monotoluene adduct at this time and was in the process of magnetically characterizing this complex and a series of related compounds (35).

Though the scope of the work in our laboratory did not extend beyond the crystal structure determination, the follow-up of the magnetic studies and their interpretations are worth mentioning. Magnetic results from three independent laboratories (36, 37, 38) concluded that $[\text{Cu}(\text{EIA})]_4$ (alpha-form) is best described magnetically by two exchange coupling constants, J_L (interaction through

Cu-Cu long bonds) and J_S (short bond interactions) with an average values of 4 and -16 cm^{-1} , respectively. This ferromagnetic and antiferromagnetic coupling, respectively, is not unusual and agrees well with the in-plane vs. out-of-plane interpretation presented by Lintvedt et.al. (39).

Interpretation of the magnetic results of the tub-like core appear to be more questionable. Haase et.al. (37) could not fit the beta-form to a susceptibility equation. However, Theriot and coworkers found overall ferromagnetic exchange constants of 15 and 10 cm to best describe the system. They attribute this overall ferromagnetic behavior to the fact that the two opposing Cu-O-Cu angles (sharing the same face of the cube) are 90 degrees (favoring ferromagnetic coupling) and 105 degrees (favoring antiferromagnetic coupling) (38). They continue their discussion by stating that the parallel pathway dominates the antiparallel exchange pathway. Since the four 90 degree Cu-O-Cu bridging angles all include longer Cu-O bonds ($2.307\text{--}2.430 \text{ \AA}$) it is difficult to envision how this effect alone could dominate the overall susceptibility of the tetramer since the antiferromagnetic bridging angles (8) include shorter Cu-O bonds ($1.976\text{--}1.946 \text{ \AA}$); the distorted cubane species is too complex to invoke such

simple bridging angle theory as the major cause of ferromagnetism. It would appear that the relative orientations of the coordination planes about each copper play a more important role in determining the magnetic properties of this system than the Cu-O-Cu angles.

The methanol solvate of the 1:1 complex of nickel and EIA was observed first in 1966 (7) but structural characterization was hampered by severe crystal decomposition problems. Up to 1976 two reasonable structural possibilities were proposed: a methanol molecule could add perpendicular to the coordination plane and yield a dimer with square pyramidal geometry about each nickel or two dimers could associate to form discrete tetramers (8).

This investigation found the complex $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_4$ to crystallize (orthorhombic space group $P2_1P2_1P2_1$, $Z=16$) into discrete, tetrameric cubane units with the neutral methanol molecule completing the octahedral coordination about each nickel (40). On the basis of the ease of desolvating this complex to the dimer, $\text{Ni}(\text{EIA})$, a tetrameric structure built-up of two bent dimeric moieties was expected. However, the cube core adopts a tub conformation, similar to the beta-form of $\text{Cu}(\text{EIA})$ but with much less distortion (long Ni-O bond dist = 2.112-2.130, short Ni-O bond dist = 2.020-2.055).

The green compound rapidly decomposes to the brown dimer, preventing variable temperature magnetic studies from being carried out on the system. Jager recorded a room temperature moment in the range of 3.2 - 3.3 BM.

N-N Bridged Complexes

Repeated attempts to prepare crystalline derivatives of a number of transition metal-DSALZ complexes failed due to the insolubility of the resulting complexes in organic solvents. The iron(III) adduct, however, was an exception and yielded beautiful dark brown crystals upon recrystallization from acetone. This was the only compound in this series which was analyzed via single crystal X-ray diffraction methods.

The structural characterization of the complex $\text{Fe}_2(\text{DSALZ})_3$ (reported herein) marks the first definitive study of a complex with this charged diiminoalcohol as a ligand. The complex maintains a dinuclear structure with a 2:3 (Fe(III):DSALZ) ratio. Each of the three ligands (binucleating) chelates to both octahedral metal centers, contributing a nitrogen and an oxygen atom to each iron atom to form the facial isomer. The slightly distorted octahedral coordination spheres about each iron(III) atom do not share a common face but rather are separated by the distance of the N-N azine bond. All structural parameters

of the ligand resulted in the values expected from the earlier structural determination (41) of the uncoordinated neutral molecule DSALZH (the uncoordinated molecule is the trans rotamer with respect to the N-N bond).

An interesting structural aspect of $\text{Fe}_2(\text{DSALZ})_3$ is the geometry about the six bridging nitrogens. They form a trigonal prism, twisted away from the eclipsed position (i.e. toward octahedral symmetry) by 24 degrees. The cobalt analog with the neutral Schiff base PMK (Figure 4; structure III), which was structurally characterized by Boyd and his group (15), also adopts a similarly distorted trigonal prismatic conformation (Figure 27; twist=17 degrees.) They convincingly reason that the twist can be attributed to the steric interactions between two bulky methyl groups. Salicylaldehyde azine (DSALZ), on the other hand, has only hydrogens in these positions. Therefore, the twist deformation probably arises from spatial requirements of the six-membered ring formed upon complexation of the ligand to the metal atom.

The magnetic moment of the dinuclear compound showed only a slight decrease (5.5 - 5.1 BM) with temperature (298 - 98 °K). This is a normal range of values for a high spin, d^5 system. If data at lower temperatures could have been obtained, it could have given more conclusive evidence

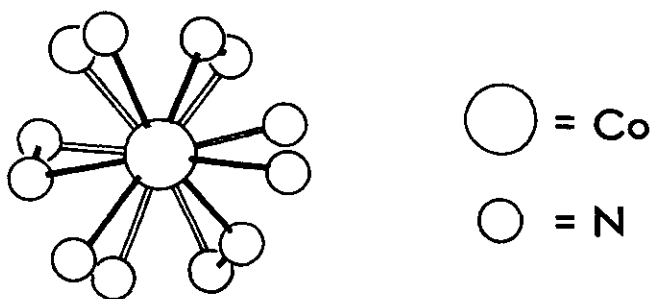


Figure 27. View Down the Co(1)-Co(2) Axis of the Coordination Sphere of $\text{Co}_2(\text{PMK})_3^{4+}$ Illustrating the Twist from Trigonal Prismatic Geometry at the N-N Azine Bonds. Unfilled Bonds Represent Co(2)-N Interactions.

about magnetic coupling within the system; the data recorded here are too far from the Néel temperature to be useful in fitting a susceptibility equation.

Dapo Complexes

The variety of hydrogen-bonded species formed by the metal complexes of 2-aminoethanol and diethanolamine prompted us to structurally investigate compounds containing the aminoalcohol 1,3-diamino-2-propanol to determine if this ligand formed analogous adducts.

The complex chosen for initial studies was an ionic Co(III) complex. Two groups (22, 23) recently formulated the cation as trans- $[\text{Co}(\text{Dapo})\text{DapoH}]^{2+}$ based on spectral

results. This was an obvious complex of choice to study hydrogen bonding since it contained both a protonated (DapoH) and deprotonated (Dapo) ligand.

The structure of the dark red crystalline needle was determined and the results confirmed that it was the trans complex, but it was revealed that it formed corner-to-corner, intermolecular hydrogen bonds (Figure 28).

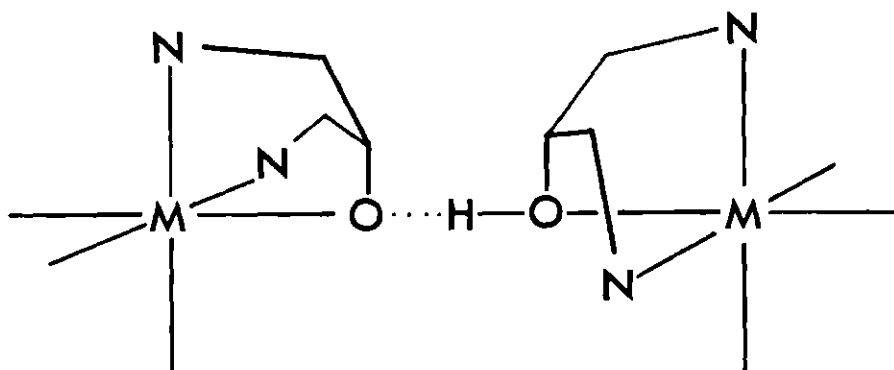


Figure 28. Corner-to-corner Hydrogen Bonding.

However, the molecules form an infinite linear chain and do not crystallize as discrete polynuclear units (Figure 29). Octahedral geometry is maintained about the cobalt center with only a very minor trigonal distortion due to the restriction of the tridentate ligand (Table 8).

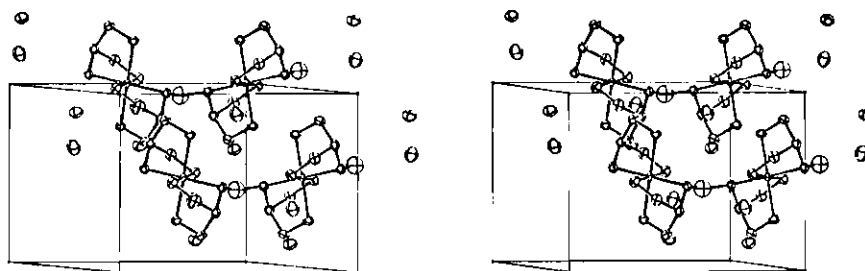


Figure 29. Stereoview of the Unit Cell and Crystal Packing of the Complex $[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$.

For an ordered structure, the hydrogen (HBND) involved in hydrogen bonding should lie directly on the two-fold axis, midway between the two oxygens. Although located at this position in a difference Fourier, upon refining the coordinates of the atom HBND, it drifted significantly away from this position, indicating a disorder in the crystal structure. To conserve the charge balance, the position of HBND was refined with an occupancy factor of 0.50. This resulted in an $\text{O}(1)\text{-HBND}$ length of 1.01 Å, an $\text{O}(1')\text{-HBND}$ bond length of 1.46 Å and an $\text{HBND} - \text{HBND}'$ dist of 0.60 Å. The observed $\text{O}(1)\text{-HBND-O}(1')$ angle is 156 degrees.

The disorder could result from a double-minimum well with the hydrogens randomly occupying either of the

minimum-energy positions between pairs of cobalt complexes. Alternatively, there could be a single, unsymmetric well with the hydrogen within one chain ordered so that each cobalt complex forms one short and one long O-H distance; the disorder in this case would result from random ordering of chain direction within the crystal.

Once the infinite chain structure of the diamagnetic Co(III) complex was determined, it was decided to prepare complexes which would be magnetically interesting and also offer different modes of intermolecular hydrogen bonding. Thus, the relatively simple d^9 -systems of copper(II) were investigated.

Initial results indicated immediate complex formation. Varying the preparative conditions, a blue, unstable crystalline material was obtained as the iodide salt. The only other results reported on this type of system was a deep blue nitrate salt which analyzed to be a 1:1:1 (Cu:Dapo: NO_3^-) complex (24). Based on the subnormal magnetic moment which it exhibited, a binuclear structure was suggested. The analysis of our iodide salt did not agree with a simple dimeric formulation. It appeared to be solvate with a whole number ratio of 3:4:4 (Cu:Dapo:I).

Preliminary results of single crystal X-ray studies concurred with a trinuclear formulation (42) and the

molecular structure was determined (Figure 30). While hydrogen bonding was initially suspected, the protonated alcohol groups do not interact with any other atoms in the unit cell (intermolecular closest approach dist $4.0 \overset{\text{O}}{\text{\AA}}$).

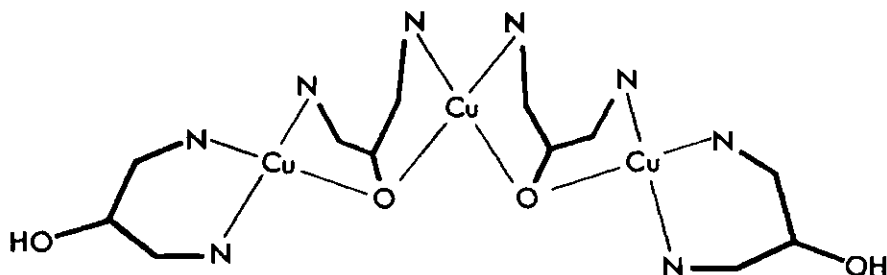


Figure 30. Schematic Diagram of the Structure of the Cation $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]^{4+}$.

Concurrent with the solution of this trinuclear structure was the publication by Näsäkkälä (25) of a complete structural study of the 1:1:1 ($\text{Cu}:\text{Dapo}:\text{NO}_3^-$) complex previously suggested to be a dimer. He unequivocally proved that it was a cyclic trimer (Figure 9) and obtained a good fit of the susceptibility equation for three coppers in an equilateral triangle. He further concluded that the complex exhibits antiferromagnetic exchange coupling (-79 cm^{-1} for the nitrate and -92 cm^{-1} for the perchlorate salt). His results are in good agreement

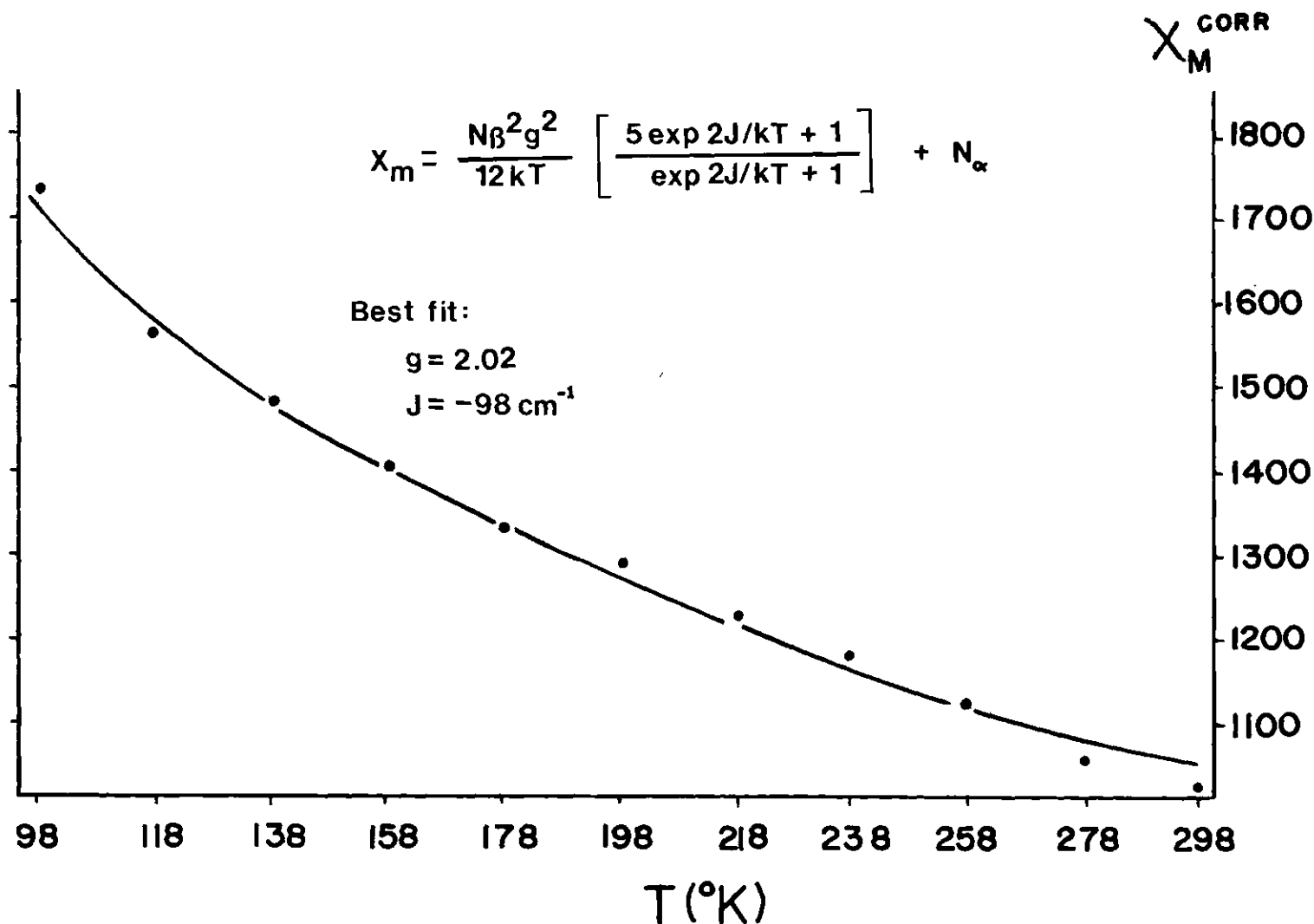


Figure 31. Graph of Molar Magnetic Susceptibility (χ_M^{corr}) vs. Temperature (°K) for $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$. Filled Circles Represent Values Observed and the Solid Line Represents Values Calculated from the Derived Equation.

with the exchange coupling constant which we obtained for the non-cyclic copper trimer ($J = -98 \text{ cm}^{-1}$). Graphic results are presented in Figure 31

Näsäkkälä's report referenced some structural parameters of a thiocyanate salt of the cation $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]^{2+}$ which were to be published. The complete report of the structure by Smolander et. al. (43) disclosed that the tetravalent cation of this thiocyanate salt adopted the same general structure as the cation of the tetraiodide salt reported in this thesis. Each copper atom in the thiocyanate salt structure is five-coordinate; Cu1 interacts with the nitrogen of a thiocyanate (Cu1-N11 dist. = 2.70 Å) whereas Cu2 and Cu3 interact with the same sulfur atom of a thiocyanate group (Cu2-S1 dist. = 2.88 Å and Cu3-S1 dist = 2.82 Å).

Although Smolander did not report any magnetic studies on the complex it would be an interesting magnetic system for comparison with the four-coordinate Cu trimer system reported herein.

Charged Diimine Complexes

The intent of this study was to prepare and structurally and magnetically characterize complexes analogous to those reported for salen by Sinn and coworkers (Figure 11). The possible pentadentate ligands (Dapac or

Dapsa) were chosen for several reasons: (1) no reports on definitive structural work for complexes of these ligands had been made, (2) the possibility of the formation of intermolecular hydrogen bonded complexes existed and (3) bi- tri- or teranuclear complexes could be formed by this ligand. Surprisingly, these ligands did not form analogs of the salen complexes but yielded a series of compounds which were quite unique.

The lack of studies in literature on complexes of Dapac and Dapsa precludes structural comparisons to complexes reported in this thesis. The magnetic properties however, can be interpreted in terms of typical dimer-like behavior.

First, a general account of these structures will be given. A short description of each specific structure will follow to more easily reference the differences between these complexes.

Each of the complexes contains two square-planar copper(II) ions bridged by both the isopropoxide oxygen and the oxygens (three atom bridge) of an acetate group. The remaining coordination sites of each copper are filled by the phenoxide oxygens and imine nitrogens of the binucleating ligands.

$\text{Cu}_2(\text{Dapac})(\text{OAc})$, crystallizes into discrete dimers and maintains a dihedral angle of 123 degrees between the distorted square-planar coordination planes of the copper atoms. The bridging Cu-O-Cu angle is 114.6 degrees. The magnetic moment shows a slight increase (1.90 - 1.97 BM) with decreasing temperature (298 - 98 °K).

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$, crystallizes into dimers which form infinite chains via corner-to-corner interactions of mutually perpendicular planes of alternating five and six-membered rings (intradimeric Cu-Cu dist interdimeric Cu-Cu bond dist.). The dimeric molecules are planar with an average dihedral angle between the copper coordination spheres of 163 degrees. The acetonitrile molecule is non-coordinating. The effective moment of the complex decreases with temperature.

$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$, crystallizes as discrete, planar dimers (avg. dihedral angle between planar coordination spheres = 169 degrees). The methanol molecule is non-coordinating. The effective moment dramatically decreases (1.71 - 0.93 BM) with temperature (298 - 98 °K), as does the molar susceptibility below 160 °K.

$\text{Cu}_2(\text{Dapsa})(\text{OAc})$, crystallizes into discrete, dimeric units (two per asymmetric unit) with a dihedral angle between coordination planes of 163 degrees. The effective moment dramatically decreases (1.68 - 1.05 BM) with temperature, as does the molar susceptibility below a temperature of 160 °K.

The observed magnetic susceptibilities of $\text{Cu}_2(\text{Dapac})(\text{OAc})$ and $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$ do not fit the dimer susceptibility equation. For $\text{Cu}_2(\text{Dapac})(\text{OAc})$, this was not expected since it exhibits ferromagnetic coupling due to

the bent nature of the dimer (39). $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$ however, does not obey the dimeric susceptibility equation due to the infinite chain interactions between each dimeric moiety. Although some theoretical models have been successfully applied to infinite chain systems (3) one could not be found which adequately described the complex interactions present in this structure. Therefore, no further attempt was made to fit the data which were recorded.

The molar magnetic susceptibilities of $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ and $\text{Cu}_2(\text{Dapsa})(\text{OAc})$ fit the dimeric susceptibility equation (Bleaney-Bower). The results are listed in Table 22. The exchange coupling constants from the fit ($J = -185 \text{ cm}^{-1}$ and $J = -159$) indicate that the complexes are strongly antiferromagnetically coupled and similar to each other. This is in good agreement with similar structures and environments which the molecules assume in the crystal structures. The slight difference in J values may arise from a combination of (a) the coordinating atoms of $\text{Cu}_2(\text{Dapsa})(\text{OAc})$ showing a larger deviation from overall planarity than those of $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ and (b) the minor difference in the Cu-O-Cu bridging angles (131 and 133 degrees respectively).

The ferromagnetically coupled complex $\text{Cu}_2(\text{Dapac})(\text{OAc})$ has a smaller Cu-O-Cu bridging angle (114.6 degrees) than the

Table 22. Magnetic Susceptibilities ($\chi_M^{\text{corr}} \times 10^6$ cgs and $\chi_{\text{calc}} \times 10^6$ cgs) of the Complexes $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ and $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.

T (°K)	χ_M^{corr}	χ_{calc}	χ_M^{corr}	χ_{calc}
	<u>$\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$</u>		<u>$\text{Cu}_2(\text{Dapsa})(\text{OAc})$</u>	
298	1226	1217	1201	1205
278	1273	1276	1237	1245
258	1343	1337	1301	1301
238	1395	1397	1355	1360
218	1461	1455	1423	1420
198	1511	1504	1483	1480
178	1540	1538	1536	1534
158	1547	1542	1568	1575
138	1486	1494	1575	1586
118	1352	1361	1517	1540
98	1101	1099	1391	1392
	$J = -185 \text{ cm}^{-1}$ $g = 1.77$ $N_\alpha = -234.2 \times 10^{-6}$		$J = -159 \text{ cm}^{-1}$ $g = 1.52$ $N_\alpha = 68.3 \times 10^{-6}$	

other complexes in this series (avg value = 132 degrees). However, based on Hodgson's correlation of bridging angle and magnetic behavior (4), this compound should be antiferromagnetically coupled (i.e. Cu-O-Cu angle 98 degrees). In this case, the non-coplanarity of the coordination spheres in the dimer apparently plays a more important role in determining the exchange mechanism.

The resulting negative value of the temperature independent paramagnetism term ($N\alpha$) of $\text{Cu}_2(\text{Dapsa})(\text{OAc})\cdot\text{CH}_3\text{OH}$ is anomalous and no explanation for this behavior can be offered at this time. The negative value appears to be adjusting the fit for diamagnetism in the system. This has not been previously observed.

The monomeric complex, $\text{Cu}(\text{DapsaH})\cdot\text{CH}_3\text{CN}$, shows large deviations from square planar geometry toward tetrahedral coordination. This is probably due to strain produced by the formation of the saturated six-membered ring upon chelation. The propylene backbone adopts a twisted conformation, and through the two imine nitrogens, distorts the geometry about the copper atom.

CHAPTER IV

CONCLUSIONS

The metal-metal distances in all complexes prepared were large enough to insure that a direct exchange mechanism via metal-metal overlap was excluded as a possible exchange mechanism. The complexes were assumed to be coupled through the bridging atoms in the polynuclear moiety.

The slight differences in the molecular structures of α -[Cu (EIA)]₄ and β -[Cu(EIA)]₄ yielded significant magnetic differences. Based on structural parameters of the tub (β -) form, the bridging angle was concluded to play a minor role in determining magnetic properties compared to the importance of the relative positions of the coordination spheres of the four copper(II) atoms.

The six bridging nitrogens of the complex $\text{Fe}_2(\text{DSALZ})_3$ were determined to show a larger distortion from trigonal prismatic geometry than the sterically hindered $\text{Co}_2(\text{PMK})_3^{4+}$. The difference may be due to the six vs five membered ring, respectively, formed upon coordination of the ligand to the metal.

The ligand Dapo was found to exhibit intermolecular hydrogen bonding in the cobalt complex

$[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$. The other Dapo-metal complex studied, $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$, revealed binucleating coordination of two monoanionic ligands, with the other two neutral ligands donating only their nitrogen atoms. The magnetic susceptibility equation for a bent trinuclear complex with no interactions between the end copper atoms gave a good fit with the experimentally observed values to yield an antiferromagnetic coupling constant ($J = -98 \text{ cm}^{-1}$).

The structural and magnetic results of the series of complexes with Dapac and Dapsa as ligands showed that: (a) in the ferromagnetically coupled complex, $\text{Cu}_2(\text{Dapac})(\text{OAc})$, the bridging angle (114.6 degrees) plays a minor role compared to that of the bent nature of the dimer in deciding the overall mechanism of exchange and, (b) the complex $\text{Cu}_2(\text{Daspa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$ is much more weakly coupled than the analogous antiferromagnetically coupled complexes of $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$ or $\text{Cu}_2(\text{Dapsa})(\text{OAc})$ due to ferromagnetic interactions in the acetonitrile solvate complex along an infinite chain.

APPENDIX

Table A. Observed (FO) and Calculated (FC) Structure Factors for $[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
H=-19				3	8	22	19	2	3	10	7	7	9	11	10	4	10	20	16	1	10	31	30	5	18	22	22	1	18	22	19
1	11	11	8	3	9	25	23	2	6	33	28	7	10	19	19	4	11	12	11	1	11	34	36	5	19	18	17	1	19	33	31
				3	12	26	24	2	7	22	25	7	12	16	12	4	12	18	9	1	13	32	30	5	21	14	13	1	21	19	17
				3	15	36	31	2	10	27	24	7	13	13	10	4	14	13	14	1	14	11	13	6	1	27	25	2	2	36	33
H=-18				3	16	21	20	2	12	39	37	H=-15				4	18	16	17	1	16	14	12	6	3	9	8	2	4	48	48
0	6	14	13	4	2	18	17	2	14	14	16	5	1	19	16	5	1	19	16	1	17	36	34	6	4	12	12	2	6	18	21
				4	4	12	8	2	16	36	36	8	2	34	31	5	4	50	46	1	20	10	5	6	5	15	14	2	7	16	13
				4	6	10	11	3	3	20	19	8	4	17	21	5	6	10	9	1	21	30	28	6	6	32	32	2	9	17	17
0	14	23	20	4	7	11	9	3	5	23	16	8	8	37	33	5	7	36	35	1	23	12	9	6	7	12	9	2	10	35	34
0	16	13	18	4	8	35	31	3	7	19	19	0	6	59	54	5	8	31	30	2	2	21	20	6	12	22	18	2	11	25	22
1	3	12	9	4	11	22	21	3	8	21	19	0	8	37	33	5	10	22	21	2	4	9	6	6	13	17	17	2	12	22	25
1	7	19	16	4	13	13	10	3	9	27	23	0	10	37	30	5	15	9	9	2	5	19	21	6	15	17	18	2	14	21	21
1	9	11	9	4	14	17	13	3	10	21	21	0	12	21	18	5	19	13	15	2	6	32	34	6	17	17	16	2	15	11	13
1	11	13	12	4	16	20	18	3	11	19	21	0	16	12	12	6	2	17	14	2	9	17	15	6	18	18	16	2	16	9	8
1	13	11	9	5	1	24	16	3	12	15	11	0	20	16	13	6	3	30	29	2	10	15	14	6	19	20	21	2	18	54	54
1	17	30	26	5	2	17	13	3	13	32	25	1	1	49	47	6	5	33	29	2	12	18	20	6	20	22	21	2	19	13	10
2	2	26	19	5	4	12	9	3	14	21	20	1	3	9	8	6	8	20	17	2	16	22	22	7	3	18	17	2	20	23	20
2	8	17	14	5	6	23	22	3	15	12	17	1	4	32	26	6	9	28	26	2	17	10	9	7	5	20	20	2	21	13	12
2	10	13	12	5	7	21	21	3	16	12	11	1	5	10	8	6	12	10	9	2	18	35	32	7	8	13	13	2	24	23	24
2	12	18	15	5	9	15	14	3	17	10	8	1	6	16	19	6	14	20	17	2	20	32	30	7	10	14	14	3	2	9	5
2	14	19	19	5	10	22	19	3	18	17	17	1	7	52	50	7	2	22	20	2	22	19	19	7	13	23	22	3	3	10	6
2	16	25	19	5	12	13	13	4	1	14	14	1	8	24	18	7	4	18	18	2	23	11	11	7	15	17	16	3	4	21	23
3	4	13	12	5	14	10	9	4	3	16	17	1	12	19	22	7	5	18	17	3	1	35	30	7	16	10	12	3	5	14	18
3	7	15	13	5	15	25	23	4	4	25	21	1	15	10	9	7	6	17	14	3	2	16	12	7	18	17	17	3	7	13	15
3	10	22	17	6	4	15	11	4	5	39	37	1	17	11	10	7	7	21	21	3	4	17	16	8	1	12	11	3	8	23	22
3	11	11	9	6	5	12	11	4	7	20	18	1	19	28	25	7	10	19	19	3	5	38	34	8	2	12	9	3	9	18	25
3	13	22	19	6	7	13	13	4	8	23	21	2	3	19	21	7	11	13	11	3	8	10	4	8	6	23	22	3	11	50	45
3	14	21	18	6	8	16	12	4	9	24	21	2	4	11	12	7	12	12	15	3	9	12	16	8	8	19	19	3	16	23	23
4	6	19	15	6	9	13	11	4	10	13	12	2	5	24	23	7	14	15	13	3	18	12	13	8	10	12	11	3	17	41	42
4	10	21	18	6	10	18	5	4	13	15	13	2	6	39	39	7	15	14	15	3	11	22	25	8	11	11	10	3	19	48	39
4	11	12	11	6	11	18	18	4	14	22	20	2	14	39	39	8	3	19	18	3	13	11	10	9	2	16	14	3	20	21	22
H=-17				4	16	12	11	2	16	20	18	2	16	20	18	8	4	14	10	3	16	16	18	9	5	25	22	3	22	19	21
H=-16				5	2	35	30	2	18	12	7	2	18	12	7	8	5	19	17	3	17	44	42	9	6	20	20	4	1	9	9
8	2	24	22	5	3	12	10	2	20	29	27	2	20	29	27	8	6	13	9	3	20	24	24	H=-13				4	2	12	16
				5	4	25	24	3	1	35	29	8	8	11	11	3	21	25	23	4	1	24	26	8	2	31	29	4	4	29	28
				5	5	24	22	3	2	23	18	8	9	10	10	4	1	24	26	4	1	24	26	8	4	12	15	4	8	15	16
8	4	10	10	5	6	32	29	3	4	12	12	8	11	13	10	4	4	28	28	4	5	15	17	8	6	30	33	4	9	17	21
8	8	35	30	5	8	34	31	3	5	10	10	3	5	10	10	4	6	36	35	4	6	31	27	0	8	58	55	4	10	18	19
8	10	11	10	5	9	20	17	3	7	46	44	H=-14				4	8	31	27	4	10	21	18	0	12	94	100	4	11	12	18
8	14	23	21	5	12	15	15	3	10	15	13	8	2	10	14	4	13	14	17	4	13	14	17	0	16	13	11	4	12	45	44
0	16	38	35	5	13	20	19	3	11	18	13	8	4	55	54	4	14	16	14	4	14	16	14	0	18	37	37	4	15	25	23
1	1	21	18	5	14	11	11	3	12	13	16	8	8	64	64	4	15	12	10	4	15	12	10	1	2	10	15	4	16	11	14
1	5	16	11	5	17	11	7	3	13	12	14	8	10	39	39	4	16	26	24	4	16	26	24	1	4	43	39	4	17	18	17
1	7	22	19	6	1	14	14	3	14	17	12	0	14	39	40	4	19	23	21	4	19	23	21	1	6	14	10	4	18	50	50
1	15	47	44	6	2	25	23	3	16	11	11	0	16	25	26	4	20	27	27	1	7	26	32	1	7	26	32	4	19	12	15
1	18	11	8	6	3	23	21	3	18	19	16	0	18	12	9	5	2	34	33	5	2	34	33	1	8	33	36	4	21	26	26
2	6	12	9	6	4	14	11	3	19	27	26	0	20	39	37	5	5	35	35	1	9	33	35	1	9	33	35	5	3	9	5
2	8	31	27	6	6	16	14	4	3	22	15	0	24	21	19	5	6	24	23	5	6	24	23	1	10	37	35	5	4	17	14
2	10	22	20	6	11	10	8	4	4	20	17	1	1	28	29	5	10	18	6	5	10	18	6	1	11	75	77	5	7	16	17
2	14	42	36	6	13	18	20	4	5	14	13	4	2	18	21	5	12	23	20	5	12	23	20	1	12	23	26	5	8	11	13
2	16	24	24	6	14	12	12	4	6	35	33	1	3	13	12	5	13	19	15	5	13	19	15	1	13	12	22	5	10	29	27
2	18	18	15	6	16	17	15	4	7	11	12	4	7	11	12	1	5	29	29	5	14	24	24	1	14	21	23	5	11	43	39
3	1	20	16	7	7	11	9	4	8	19	18	1	6	35	37	5	16	12	8	5	16	12	8	1	16	11	14	5	12	15	16
3	2	11	7	7	8	20	27	4	9	24	25	1	7	34	42	5	17	22	20	5	17	22	20	1	17	28	27	5	14	46	43

Table A. (continued)

K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC
5	16	36	36	H--12				3	12	18	21	6	18	12	10	0	6	8	18	3	11	78	70	7	3	28	30	11	6	24	24
5	17	14	15					3	13	51	52	6	19	10	18	0	8	24	21	3	13	27	26	7	4	37	37	11	8	26	24
5	18	15	14	0	2	57	58	3	14	22	19	6	20	20	21	0	10	109	114	3	15	22	26	7	5	9	9				
5	19	26	25	0	4	27	28	3	15	17	19	7	1	15	17	0	12	57	95	3	16	20	19	7	6	33	31	H--10			
5	20	27	30	0	6	18	15	3	17	24	28	7	2	18	19	0	14	13	10	3	17	36	34	7	7	13	10	0	2	79	41
5	22	13	16	0	8	45	47	3	18	23	26	7	3	22	22	0	16	57	59	3	20	12	12	7	8	55	54	0	4	98	99
6	2	22	21	0	10	107	109	3	19	32	30	7	4	24	25	0	18	36	39	3	25	11	14	7	9	14	11	0	6	18	12
6	4	33	31	0	12	55	53	3	20	14	13	7	5	30	30	0	20	36	38	4	1	15	12	7	11	17	13	0	8	48	50
6	6	10	15	0	14	43	40	3	21	14	12	7	6	35	34	0	22	42	37	4	2	29	32	7	12	40	40	0	12	72	75
6	7	24	24	0	16	47	40	3	22	14	14	7	8	18	17	1	1	48	52	4	3	13	15	7	15	33	31	0	14	30	37
6	9	10	9	0	18	16	16	3	23	19	19	7	9	34	31	1	2	12	14	4	4	49	55	7	16	12	10	0	16	45	45
6	10	31	32	0	20	16	21	4	1	16	17	7	10	39	37	1	3	98	102	4	5	11	13	7	17	27	30	0	18	21	26
6	11	21	20	0	22	30	26	4	2	10	11	7	12	15	17	1	4	38	37	4	6	10	9	0	1	23	22	0	20	44	52
6	14	16	14	0	24	22	23	4	4	15	19	7	14	9	4	1	5	64	64	4	7	64	63	0	2	37	39	0	22	15	14
6	15	42	42	1	2	62	65	4	5	23	19	7	16	11	11	1	6	19	18	4	8	55	51	0	3	33	33	0	24	43	58
6	16	28	26	1	3	68	73	4	6	8	14	7	17	27	28	1	7	27	28	4	9	50	52	0	4	46	45	0	26	11	11
6	17	14	14	1	4	9	6	4	7	31	35	7	18	29	31	1	8	16	18	4	10	70	67	0	5	46	45	1	1	144	149
6	18	25	27	1	6	38	38	4	8	11	18	7	19	16	18	1	9	68	68	4	11	34	35	0	6	35	35	1	2	58	68
6	19	16	18	1	7	28	28	4	10	35	31	8	1	14	16	1	10	46	45	4	12	17	17	0	7	22	22	1	3	10	24
6	21	28	28	1	8	29	28	4	11	30	33	8	2	22	23	1	11	96	98	4	14	10	11	0	8	12	20	1	4	16	14
7	1	15	14	1	9	97	97	4	12	63	60	8	3	13	13	1	12	17	23	4	16	27	27	0	9	23	24	1	5	78	95
7	3	15	14	1	12	55	56	4	13	30	26	8	4	38	39	1	14	58	57	4	17	23	24	0	10	17	15	1	6	28	32
7	4	16	13	1	13	63	61	4	14	28	27	8	5	31	31	1	15	18	14	4	18	20	21	0	11	14	17	1	7	45	55
7	5	15	15	1	14	30	27	4	15	13	9	8	7	21	25	1	16	20	26	4	20	25	29	0	12	14	15	1	8	45	48
7	6	19	19	1	15	20	19	4	16	34	35	8	8	15	15	1	17	54	50	5	22	19	16	0	13	21	22	1	9	30	36
7	7	18	20	1	16	21	19	4	17	36	35	8	9	19	19	1	18	26	28	5	1	24	27	0	14	13	14	1	10	69	67
7	8	33	31	1	17	28	26	4	18	23	21	8	10	37	33	1	20	23	22	5	2	21	24	9	1	13	15	1	11	28	32
7	11	22	22	1	19	26	25	4	19	17	15	8	11	33	33	1	21	13	10	5	3	44	40	9	2	20	18	1	12	28	32
7	12	13	13	1	20	22	23	4	20	24	27	8	13	10	9	1	22	17	17	5	6	10	13	9	3	23	23	1	13	52	48
7	13	16	15	1	23	11	8	4	24	21	18	8	16	15	14	1	23	24	29	5	7	25	28	9	4	17	15	1	14	32	38
7	15	10	9	2	2	66	69	5	1	16	18	8	17	25	24	1	24	16	17	5	8	37	36	9	5	39	39	1	15	25	28
7	16	32	31	2	3	18	19	5	3	15	17	8	19	18	17	1	25	11	12	5	9	18	22	9	6	10	6	1	16	46	47
7	19	16	18	2	4	36	37	5	5	28	27	9	1	15	16	2	1	49	57	5	10	58	58	9	7	11	8	1	17	24	27
8	1	12	12	2	6	43	50	5	6	12	12	9	2	20	21	2	3	16	19	5	11	49	50	9	8	33	35	1	18	38	36
8	2	18	17	2	7	15	13	5	8	11	8	9	4	19	21	2	4	128	142	5	12	21	20	9	9	23	23	1	19	11	17
8	3	14	13	2	8	71	70	5	9	45	44	9	5	31	33	2	5	11	13	5	13	18	16	9	10	25	22	2	2	136	148
8	4	28	27	2	9	9	13	5	11	18	18	9	7	28	27	2	6	45	46	5	14	58	50	9	11	14	16	2	3	30	35
8	6	33	31	2	10	26	24	5	12	63	63	9	8	20	21	2	7	22	23	5	16	15	17	9	12	15	17	2	4	40	45
8	7	16	13	2	11	43	43	5	13	37	37	9	10	19	16	2	8	24	22	5	17	28	26	9	14	28	29	2	5	8	13
8	8	12	12	2	12	77	76	5	16	54	55	9	12	36	37	2	9	38	36	5	18	30	31	9	15	22	22	2	6	68	78
8	9	18	18	2	13	44	39	5	17	24	24	9	14	10	10	2	10	113	107	6	1	29	33	9	17	21	21	2	7	11	17
8	12	13	10	2	15	19	19	5	18	23	24	9	16	24	23	2	13	29	29	6	2	12	9	10	1	21	22	2	8	70	76
8	13	10	7	2	16	48	49	5	19	24	25	10	1	12	7	2	15	43	44	6	3	26	30	10	2	12	12	2	9	29	28
8	14	12	7	2	17	24	27	5	23	16	18	10	2	12	10	2	16	36	39	6	4	39	40	10	4	9	9	2	12	45	44
8	15	18	17	2	20	37	36	6	1	11	14	10	3	18	18	2	21	11	14	6	5	8	9	10	5	11	11	2	13	33	29
8	17	23	23	2	21	10	12	6	2	25	29	10	5	10	8	2	24	11	11	6	7	29	28	10	6	15	14	2	15	9	18
9	3	24	23	2	22	13	14	6	5	11	11	10	6	12	10	2	25	17	16	6	8	35	35	10	7	18	16	2	16	50	49
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9	7	19	17	3	3	40	40	6	8	35	32	10	11	26	23	3	2	46	42	6	12	14	16	10	9	28	28	2	18	18	19
9	9	15	15	3	4	31	34	6	11	45	41	10	12	15	13	3	3	86	90	6	13	52	50	10	12	18	17	2	19	12	14
9	10	21	19	3	5	28	31	6	12	29	30	10	13	22	23	3	5	46	50	6	15	12	9	10	13	22	20	2	20	20	23
9	13	13	11	3	6	49	52	6	13	29	30	3	6	63	60	3	6	63	60	6	16	19	15	10	14	15	10	2	24	14	22
9	14	24	22	3	7	12	15	6	14	24	26	3	7	22	21	3	7	22	21	6	17	23	23	11	1	10	11	2	26	10	10
10	4	22	21	3	9	53	53	6	15	22	19	3	8	66	71	3	8	66	71	6	18	33	34	11	2	20	18	3	1	128	131
10	9	11	13	3	10	37	39	6	16	17	15	0	2	90	91	3	9	43	44	7	1	16	15	11	4	10	11	3	2	20	25
				3	11	39	41	6	17	36	36	0	4	74	76	3	10	10													

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
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3	5	56	56	6	8	56	59	10	13	13	9	2	12	67	66	5	14	10	7	8	12	12	18	1	3	18	12	3	23	38	48
3	6	24	31	6	9	13	11	10	14	16	15	2	13	50	50	5	15	24	29	8	13	34	32	1	4	27	29	4	1	26	29
3	7	27	27	6	10	24	23	10	16	31	30	2	14	105	99	5	16	18	13	8	14	20	18	1	5	74	85	4	2	53	54
3	8	66	64	6	11	29	31	11	4	34	35	2	16	31	32	5	17	16	17	8	16	35	35	1	6	16	8	4	3	16	18
3	9	69	66	6	12	12	15	11	6	14	13	2	17	10	16	5	18	25	26	8	17	23	23	1	8	80	81	4	4	35	36
3	10	35	39	6	13	32	30	11	7	18	14	2	19	16	13	5	19	13	18	8	19	22	22	1	10	29	25	4	5	16	17
3	11	43	38	6	14	21	19	11	8	17	15	2	20	29	30	5	20	34	36	9	3	11	14	1	11	62	63	4	6	140	147
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3	13	15	14	6	16	42	37	2	24	15	18	5	24	36	39	5	24	36	39	9	6	10	10	1	13	135	141	4	8	72	78
3	14	10	11	6	17	18	21	2	25	16	14	6	1	24	27	9	7	59	55	9	7	59	55	1	15	97	95	4	9	37	37
3	16	22	22	6	19	12	8	3	1	11	20	6	2	17	19	9	9	12	12	9	9	12	12	1	16	27	31	4	10	28	25
3	21	25	24	6	21	23	21	0	2	147	157	3	2	33	36	6	3	59	62	9	10	18	6	1	17	67	69	4	11	45	43
3	23	28	30	6	23	21	24	0	4	30	26	3	3	68	73	6	4	43	45	9	11	19	19	1	18	25	22	4	12	43	48
3	24	19	16	7	1	14	18	0	6	36	37	3	4	21	17	6	5	26	27	9	12	10	9	1	19	59	60	4	13	26	25
4	1	15	15	7	4	55	55	0	8	22	22	3	5	40	40	6	6	33	32	9	13	10	10	1	20	25	26	4	15	54	52
4	2	45	51	7	5	9	10	0	10	50	54	3	6	79	80	6	8	21	22	9	17	33	34	1	22	24	27	4	16	16	15
4	3	44	46	7	6	29	29	0	12	14	18	3	7	39	37	6	10	20	18	9	18	12	11	1	23	48	52	4	17	16	28
4	4	63	56	7	8	44	48	0	14	77	75	3	8	18	15	6	12	38	39	9	19	16	17	2	1	36	43	4	19	32	31
4	5	48	49	7	9	30	31	0	16	17	13	3	9	32	26	6	13	14	20	10	1	33	30	2	2	67	71	4	20	51	54
4	6	51	53	7	10	31	33	0	18	37	35	3	10	48	51	6	14	38	37	10	3	10	9	2	3	17	11	4	22	37	41
4	7	25	22	7	12	27	25	0	20	19	28	3	12	63	60	6	15	16	15	10	5	11	8	2	4	16	18	4	24	23	22
4	8	64	64	7	13	18	13	0	22	77	79	3	14	57	56	6	16	10	5	10	10	18	18	2	5	8	5	5	1	44	54
4	9	50	50	7	15	35	36	0	24	16	17	3	15	69	71	6	18	13	12	10	11	11	13	2	6	7	6	5	2	27	34
4	10	60	54	7	16	16	17	0	26	11	13	3	16	35	38	6	19	41	41	10	12	15	16	2	8	27	23	5	3	22	21
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4	20	37	36	8	3	29	30	1	6	27	30	4	3	7	3	7	3	25	23	11	6	21	22	2	14	48	47	5	10	24	28
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4	24	30	28	8	5	44	42	1	8	18	17	4	5	54	57	7	5	12	10	11	9	17	18	2	18	55	54	5	12	47	48
5	1	56	56	8	6	53	52	1	9	20	20	4	7	15	16	7	6	48	38	11	12	17	17	2	19	19	21	5	13	45	47
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5	4	23	27	8	9	46	46	1	11	31	34	4	9	24	25	7	9	13	11	12	3	13	12	2	21	32	36	5	16	14	13
5	5	19	19	8	10	34	36	1	12	11	13	4	10	65	64	7	10	19	20	12	4	21	21	2	22	49	50	5	18	19	19
5	7	15	22	8	14	11	12	1	13	33	35	4	13	49	45	7	12	14	14	12	7	18	16	2	26	14	18	5	19	32	34
5	8	12	14	8	15	13	15	1	14	18	20	4	14	29	24	7	13	21	25	12	8	20	19	3	1	82	92	5	20	16	16
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5	18	19	22	8	18	28	29	1	16	27	29	4	16	22	19	7	15	25	24	3	3	55	56	5	3	55	56	5	23	29	38
5	11	26	26	9	2	36	38	1	18	15	20	4	17	32	34	7	16	11	11	3	4	54	60	6	1	59	68	6	1	59	68
5	12	27	25	9	3	22	22	1	20	29	28	4	18	27	29	7	17	35	36	8	2	34	38	3	5	51	51	6	2	70	71
5	14	34	30	9	4	18	20	1	21	59	65	4	19	28	31	7	18	35	33	8	4	48	33	3	8	19	16	6	3	14	15
5	15	15	11	9	7	36	34	1	23	15	17	4	22	53	57	7	19	11	11	0	6	73	81	3	9	39	41	6	5	23	22
5	16	17	22	9	9	42	41	1	24	17	19	4	24	12	13	7	20	13	11	0	8	52	53	3	10	35	38	6	7	37	38
5	17	11	13	9	10	23	22	1	25	10	16	4	25	19	18	7	21	14	15	0	10	8	7	3	11	14	11	6	8	41	34
5	18	27	22	9	11	11	11	2	1	35	42	5	1	21	24	8	1	28	32	0	12	104	99	3	12	28	25	6	9	60	61
5	21	19	21	9	12	17	13	2	2	61	78	5	2	42	42	8	2	28	29	0	14	8	4	3	13	117	117	6	10	58	56
5	22	35	33	9	15	28	27	2	3	17	21	5	3	40	41	8	3	10	14	0	16	74	75	3	14	65	69	6	12	44	45
5	23	29	29	10	1	10	10	2	4	56	59	5	4	63	68	8	4	32	30	0	18	81	87	3	15	51	51	6	13	16	28
5	24	16	19	10	2	20	20	2	5	12	11	5	5	27	29	8	5	21	18	0	20	46	49	3	16	29	29	6	14	17	18
6	1	14	14	10	3	28	29	2	7	11	11	5	6	19	13	8	6	19	16	0	22	53	46	3	17	22	23	6	15	25	21
6	2	40	41	10	5	19	18	2	8	29	27	5	7	93	99	8	7	12	11	0	24	14	22	3	18	33	35	6	16	42	43
6	3	40	43	10	6	19	20	2	9	21	21	5	9	42	43	8	8	38	35	0	26	12	15	3	19	40	41	6	17	21	21
6	4	13	12	10	9	14	13	2	10	34	40	5	10	50	53	8	9	17	19	1	1	57									

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
6	20	18	18	10	7	15	17	1	24	14	14	4	16	18	20	7	18	31	29	12	3	27	24	2	16	22	28	5	8	125	128
6	21	33	32	10	8	33	35	1	25	17	17	4	17	42	44	7	21	33	33	12	4	19	18	2	18	33	30	5	7	70	64
6	22	18	17	10	9	13	9	2	1	42	41	4	18	50	49	8	1	11	13	12	5	10	4	2	19	21	26	5	8	133	138
6	24	14	12	10	10	36	33	2	2	20	26	4	20	39	42	8	2	35	33	12	6	12	12	2	21	10	11	5	9	31	21
7	1	48	58	10	12	11	10	2	3	29	34	4	22	28	33	8	3	25	27	12	7	10	10	2	22	11	9	5	10	48	38
7	2	8	10	10	13	26	25	2	4	8	6	4	24	10	10	8	4	28	28	12	8	16	15	2	24	39	43	5	11	67	68
7	3	11	7	10	15	18	19	2	5	11	16	5	1	19	21	8	5	40	40	12	10	16	17	2	26	33	38	5	12	69	64
7	4	12	10	10	16	14	13	2	6	56	57	5	2	87	94	8	6	62	68	12	11	14	16	3	1	53	57	5	13	21	14
7	5	16	16	10	17	11	11	2	7	15	17	5	3	66	72	8	7	26	25	3	2	38	48	5	15	23	20	5	15	23	20
7	6	13	13	11	1	29	30	2	8	20	19	5	4	64	67	8	9	24	22	3	3	82	77	5	16	12	18	5	16	12	18
7	7	35	32	11	4	19	21	2	9	71	70	5	6	115	117	8	10	21	19	3	4	136	125	5	17	19	21	5	17	19	21
7	8	13	14	11	7	21	21	2	10	86	83	5	7	119	118	8	11	49	50	3	5	210	215	5	19	48	51	5	19	48	51
7	9	11	10	11	10	17	15	2	11	43	48	5	8	37	35	8	13	32	31	3	6	61	60	5	22	10	15	5	22	10	15
7	10	26	30	11	11	25	24	2	14	201	198	5	9	8	9	8	15	37	35	3	7	62	67	5	24	14	14	5	24	14	14
7	11	13	15	11	14	26	26	2	15	14	25	5	10	104	105	8	16	25	25	3	8	28	36	6	1	73	78	6	1	73	78
7	12	20	19	12	1	11	8	2	17	24	25	5	11	45	42	8	17	37	36	3	10	51	48	6	2	34	37	6	2	34	37
7	13	20	21	12	3	10	10	2	18	12	9	5	12	19	19	8	18	47	44	3	11	106	104	6	3	95	99	6	3	95	99
7	14	52	49	12	5	23	20	2	19	24	27	5	13	61	58	8	19	19	20	3	12	15	19	6	4	32	34	6	4	32	34
7	15	37	36	12	6	20	19	2	20	49	54	5	14	14	20	8	20	22	22	3	13	56	56	6	5	52	52	6	5	52	52
7	16	24	27	12	8	21	19	2	21	12	12	5	16	14	15	8	22	15	17	3	14	58	59	6	6	35	37	6	6	35	37
7	18	11	14	12	10	12	12	2	26	23	25	5	18	27	26	9	1	18	19	3	15	76	75	6	7	112	118	6	7	112	118
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7	22	13	14	3	3	64	68	3	3	64	68	5	22	20	20	9	6	39	40	3	19	49	48	6	11	57	55	6	11	57	55
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8	9	26	26	3	10	18	12	3	10	18	12	6	6	55	55	9	14	18	12	4	1	45	50	7	1	41	42	7	1	41	42
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8	11	21	20	3	12	72	73	3	12	72	73	6	8	50	54	9	17	10	6	4	3	38	43	7	3	12	15	7	3	12	15
8	13	31	29	3	13	107	98	3	13	107	98	6	9	54	51	9	18	23	24	4	4	160	166	7	4	30	31	7	4	30	31
8	14	15	17	3	15	62	63	3	15	62	63	6	10	59	51	9	19	18	18	4	5	86	89	7	5	63	68	7	5	63	68
8	15	36	42	3	16	74	70	3	16	74	70	6	11	72	70	9	20	14	15	4	6	114	113	7	6	74	76	7	6	74	76
8	18	21	23	3	17	10	17	3	17	10	17	6	12	20	21	10	2	48	36	4	7	63	96	7	7	56	52	7	7	56	52
8	19	18	18	3	18	32	35	3	18	32	35	6	13	16	16	10	5	21	21	4	8	129	126	7	8	41	41	7	8	41	41
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8	21	23	26	3	21	48	51	3	21	48	51	6	15	9	10	10	8	53	50	4	10	58	53	7	10	29	27	7	10	29	27
9	1	20	29	3	23	18	14	3	23	18	14	6	17	15	19	10	9	27	25	4	11	13	17	7	11	17	19	7	11	17	19
9	3	18	20	3	24	11	12	3	24	11	12	6	19	11	14	10	11	37	37	4	12	68	71	7	12	10	9	7	12	10	9
9	4	19	15	3	25	15	17	3	25	15	17	6	20	26	22	10	12	29	26	4	13	68	71	7	13	13	15	7	13	13	15
9	5	27	25	4	1	24	23	4	1	24	23	6	23	16	17	10	14	20	19	4	14	44	40	7	14	58	59	7	14	58	59
9	7	43	42	4	2	9	14	4	2	9	14	7	2	36	37	10	16	17	19	4	16	38	41	7	16	19	28	7	16	19	28
9	8	24	21	4	3	15	18	4	3	15	18	7	3	15	14	10	17	19	17	4	17	24	28	7	17	47	48	7	17	47	48
9	9	36	36	4	4	163	176	4	4	163	176	7	4	60	57	11	2	17	17	4	18	21	20	7	18	21	22	7	18	21	22
9	11	15	13	4	5	23	29	4	5	23	29	7	5	30	31	11	3	22	22	4	19	20	19	7	19	20	19	7	19	20	19
9	12	21	20	4	6	109	110	4	6	109	110	7	6	20	21	11	4	11	12	4	20	51	54	8	1	50	54	8	1	50	54
9	14	21	24	4	7	28	28	4	7	28	28	7	7	57	59	11	6	12	9	4	22	21	21	8	2	27	26	8	2	27	26
9	15	24	24	4	8	82	79	4	8	82	79	7	9	17	17	11	9	38	43	4	24	11	15	8	3	28	38	8	3	28	38
9	16	15	13	4	9	41	40	4	9	41	40	7	10	34	34	11	11	27	27	4	25	12	15	8	4	36	38	8	4	36	38
9	17	28	27	4	11	38	35	4	11	38	35	7	11	13	18	11	12	31	31	4	26	1	6	8	5	27	23	8	5	27	23
9	18	13	12	4	12	18	21	4	12	18	21	7	12	56	57	11	14	14	11	4	27	19	20	8	6	25	23	8	6	25	23
9	20	20	21	4	13	33	38	4	13	33	38	7	13	25	25	11	15	11	10	4	28	42	39	8	7	79	88	8	7	79	88
10	2	32	35	4	14	66	65	4	14	66	65	7	14	13	8	12	1	18	18	4	29	4	58	8	8	35	88	8	8	35	88
10	4	20	20	4	15	37	37	4	15	37	37	7	16	40	42	12															

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
8	10	12	13	13	4	15	11	2	22	36	36	5	13	51	47	8	15	9	11					3	2	18	22	5	14	57	54				
8	12	13	13	13	5	16	14	2	24	52	56	5	15	28	24	8	18	31	31					3	3	113	107	5	15	35	29				
8	13	44	45	13	6	16	15	2	26	20	24	5	16	44	41	8	20	44	45					3	4	108	111	5	16	60	66				
8	14	14	11					3	1	69	70	5	17	47	46	9	1	21	25					3	5	37	39	5	17	18	23				
8	15	13	19					3	2	159	170	5	18	12	12	9	2	11	15					3	6	57	58	5	18	57	68				
8	16	36	36					3	3	106	110	5	20	32	34	9	3	50	52					3	7	105	91	5	19	46	50				
8	18	28	27					3	4	26	19	5	24	12	10	9	4	47	45					3	8	42	46	5	22	22	24				
8	19	17	17					3	5	149	145	5	25	26	27	9	5	17	17					3	9	25	27	5	23	30	34				
8	20	29	29					3	6	98	85	6	1	8	6	9	6	37	35					3	10	117	117	5	24	12	17				
8	22	21	21					3	7	59	50	6	2	15	21	9	7	16	13					3	11	113	109	6	1	72	68				
9	2	20	23					3	8	50	53	6	3	152	156	9	8	51	52					3	12	23	32	6	2	28	26				
9	4	19	21					3	9	13	13	6	4	34	37	9	10	41	43					3	13	43	46	6	3	35	36				
9	5	43	42					3	10	30	26	6	5	106	108	9	11	21	17					3	14	16	16	6	4	49	51				
9	6	56	58					3	11	19	19	6	6	55	60	9	12	10	9					3	15	60	55	6	5	78	72				
9	7	66	65					3	12	55	52	6	7	29	22	9	13	23	23					3	17	45	47	6	6	11	18				
9	8	57	55					3	13	95	100	6	8	27	25	9	14	9	5					3	19	46	48	6	7	29	31				
9	9	20	19					3	15	66	68	6	9	71	68	9	16	18	19					3	20	40	42	6	8	99	97				
9	10	10	7					3	16	37	38	6	10	110	106	9	17	35	31					3	23	49	53	6	9	10	18				
9	11	17	16					3	17	59	54	6	12	30	25	9	19	21	20					3	24	26	31	6	10	36	37				
9	12	39	38					3	18	14	13	6	13	27	28	9	20	12	14					3	25	27	31	6	11	10	4				
9	13	11	8					3	19	30	32	6	14	25	21	10	2	9	10					4	1	97	93	6	12	66	59				
9	17	17	18					3	20	12	15	6	16	10	8	10	3	32	33					4	2	58	57	6	13	41	39				
9	19	40	43					3	22	28	31	6	17	17	19	10	4	13	13					4	3	75	64	6	14	29	28				
9	20	16	17					3	25	43	48	6	20	15	18	10	5	43	40					4	4	229	227	6	15	12	11				
10	1	21	22					4	1	31	24	6	21	26	31	10	8	46	42					4	5	74	64	6	16	17	22				
10	2	10	8					4	2	127	139	6	23	14	15	10	9	40	38					4	6	21	10	6	17	57	61				
10	3	20	21					4	3	171	167	6	24	25	32	10	10	64	65					4	7	21	16	6	19	40	43				
10	4	17	16					4	4	113	104	7	1	36	39	10	11	18	19					4	8	28	29	6	21	14	17				
10	5	11	10					4	6	229	227	7	2	121	125	10	14	34	35					4	9	24	14	6	22	31	34				
10	6	32	33					4	7	57	62	7	3	27	27	10	18	11	6					4	10	7	6	6	23	18	24				
10	7	47	46					4	8	33	32	7	4	88	90	11	1	28	28					4	11	23	25	7	1	34	36				
10	9	19	16					4	9	63	63	7	5	48	47	11	2	29	28					4	12	21	20	7	2	23	23				
10	10	42	44					4	10	35	25	7	6	23	22	11	4	14	16					4	13	25	26	7	3	17	18				
10	11	32	29					4	11	43	42	7	7	16	16	11	7	25	22					4	14	9	10	7	4	78	75				
10	12	39	36					4	12	30	36	7	9	32	32	11	8	18	16					4	15	9	14	7	5	31	32				
10	13	32	30					4	13	31	33	7	10	18	13	11	9	22	19					4	16	109	113	7	6	10	5				
10	15	13	14					4	14	23	22	7	11	27	28	11	10	14	15					4	17	34	33	7	7	9	9				
11	1	32	27					4	16	10	10	7	12	39	38	11	11	44	44					4	18	57	62	7	9	58	53				
11	2	11	15					4	18	96	100	7	13	27	27	11	12	28	26					4	19	40	44	7	10	48	45				
11	3	14	16					4	19	15	22	7	14	13	14	11	13	33	32					4	20	35	39	7	10	49	45				
11	4	15	15					4	20	28	27	7	16	13	10	11	16	16	15					4	22	16	20	7	11	72	65				
11	5	11	10					4	21	25	26	7	17	19	23	12	1	23	18					4	23	25	25	7	12	26	21				
11	7	34	34					4	23	20	23	7	19	31	34	12	3	27	23					4	25	13	21	7	14	23	19				
11	9	40	41					4	24	17	22	7	22	28	28	12	4	26	24					5	1	60	55	7	17	14	16				
11	10	19	19					5	1	13	5	8	1	28	31	12	6	22	21					5	2	84	83	7	18	26	29				
11	12	12	15					5	2	55	49	8	2	8	7	12	10	23	23					5	3	86	90	7	20	25	26				
11	13	20	19					5	3	103	112	8	3	75	67	12	11	24	23					5	4	36	34	7	21	16	14				
11	14	36	35					5	4	174	183	8	4	64	64	12	13	16	15					5	5	111	111	7	23	15	19				
11	16	17	14					5	5	76	69	8	5	45	44	13	1	35	35					5	6	67	59	8	1	43	40				
12	1	26	23					5	6	53	44	8	6	68	66	13	2	11	10					5	7	30	36	8	2	94	88				
12	2	36	31					5	7	100	100	8	7	28	27	13	3	31	30					5	8	11	6	8	3	23	18				
12	5	20	18					5	8	104	95	8	8	31	29	13	4	22	22					5	9	44	43	8	4	101	94				
12	8	12	12					5	9	36	37	8	9	29	27	13	6	13	15					5	10	12	11	8	5	32	27				
12	9	11	15					5	10	43	45	8	11	20	24	13	7	16	17					5	11	61	58	8	6	15	12				
12	10	22	23					5	11	28	30	8	13	10	9	2	26	49	54					5	12	23	26	8	9	16	18				
13	3	22	20					5	12	24	27	8	14	9	12	3	1	8	1					5	13	18	19	8	10	24	21				

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
8	11	30	28	13	2	26	24	2	19	19	24	5	16	51	51	8	16	27	29	13	4	23	28	2	17	17	16	5	15	94	89				
8	14	9	10	13	4	11	11	2	20	24	21	5	17	74	81	8	17	13	14	13	5	22	22	2	18	29	27	5	16	98	102				
8	16	29	31	13	5	21	19	2	24	68	70	5	18	53	55	8	19	16	17	13	5	22	22	2	22	51	54	5	17	20	32				
8	17	23	23	13	6	18	16	3	1	39	46	5	19	10	18	8	20	12	14	N = -2				2	24	14	16	5	18	29	33				
8	18	42	42	13	8	12	12	3	2	46	52	5	20	56	59	8	21	33	33	2	26	11	14	5	20	14	21	5	20	14	21				
8	19	24	26	M = -3				3	3	28	25	5	23	24	24	9	1	24	26	3	1	75	78	5	23	12	15	5	23	12	15				
8	20	11	8	M = -3				3	4	100	95	5	25	16	13	9	2	46	42	0	2	87	51	3	2	66	57	6	3	37	48				
9	1	56	53	M = -3				3	5	39	44	6	2	16	13	9	3	75	69	0	4	156	142	3	3	16	9	6	4	9	6				
9	2	25	22	8	2	207	233	3	6	63	51	6	4	40	41	9	4	37	36	6	6	28	33	3	4	25	23	6	5	71	71				
9	4	36	34	M = -3				3	7	87	86	6	5	12	10	9	5	65	64	6	6	28	33	3	5	8	8	6	7	23	21				
9	5	49	52	8	4	125	115	3	8	153	146	6	6	48	46	9	6	45	41	8	8	140	123	3	6	113	112	6	8	153	148				
9	6	50	47	8	6	93	102	3	9	111	95	6	7	8	10	9	9	34	31	0	10	87	60	3	7	116	119	6	9	70	67				
9	7	22	21	8	8	52	62	3	10	108	87	6	8	12	15	9	10	23	22	0	12	54	50	3	8	50	36	6	10	69	64				
9	8	21	21	0	10	124	122	3	12	71	69	6	9	30	28	9	11	13	16	0	14	167	161	3	9	43	74	6	11	68	67				
9	9	19	19	0	12	57	57	3	14	39	36	6	10	107	107	9	12	11	9	0	16	70	59	3	10	171	152	6	12	31	29				
9	10	9	10	0	14	100	99	3	15	13	12	6	12	36	35	9	13	17	14	0	18	78	74	3	11	69	71	6	13	75	75				
9	11	32	32	0	16	138	132	3	17	106	105	6	13	29	29	9	14	40	41	0	20	23	20	3	14	63	57	6	15	34	35				
9	12	13	13	0	18	45	51	3	20	29	28	6	14	22	19	9	15	15	15	0	24	15	15	3	15	94	93	6	17	56	56				
9	14	33	30	0	22	16	14	3	21	11	15	6	15	81	82	9	16	42	44	0	26	13	12	3	16	9	19	6	22	38	44				
9	15	13	8	0	24	40	39	3	22	27	29	6	16	12	14	9	17	22	26	1	1	149	136	3	17	32	32	7	1	14	16				
9	16	15	16	0	26	11	14	3	23	30	34	6	19	53	55	9	18	12	12	1	2	44	63	3	19	14	16	7	2	31	29				
9	17	13	10	1	1	89	87	3	25	21	25	6	20	12	15	9	19	20	27	1	3	132	83	3	20	18	16	7	3	60	63				
9	18	34	38	1	2	97	90	3	26	12	17	6	21	24	28	9	20	28	29	1	4	39	27	3	23	27	29	7	4	74	67				
9	19	20	23	1	3	15	35	4	1	13	26	6	24	36	36	10	1	10	13	1	5	193	155	3	25	24	25	7	5	58	68				
10	1	34	31	1	4	130	121	4	2	155	151	7	1	14	8	10	2	15	16	1	6	132	130	4	1	11	25	7	6	95	89				
10	2	12	13	1	5	72	78	4	3	35	27	7	2	17	14	10	4	14	12	1	7	77	69	4	2	93	85	7	7	35	39				
10	3	22	25	1	6	63	68	4	4	12	7	7	3	29	27	10	5	37	36	1	8	27	35	4	3	15	5	7	8	45	45				
10	4	9	9	1	7	158	151	4	5	68	65	7	4	51	50	10	7	19	18	1	9	117	109	4	4	40	47	7	9	27	25				
10	6	12	11	1	8	112	95	4	6	47	49	7	5	40	40	10	9	15	13	1	11	126	123	4	5	41	41	7	10	121	114				
10	7	26	23	1	9	61	48	4	7	120	102	7	6	59	67	10	10	50	49	1	12	98	94	4	6	56	48	7	11	38	48				
10	8	59	56	1	10	52	55	4	8	38	33	7	8	87	83	10	11	11	13	1	13	66	58	4	7	18	24	7	12	49	46				
10	10	15	13	1	11	83	76	4	9	87	80	7	9	92	91	10	12	43	43	1	14	19	26	4	8	178	167	7	14	27	21				
10	12	49	47	1	12	45	45	4	10	89	88	7	11	12	11	10	13	13	13	1	15	132	133	4	9	14	12	7	15	23	21				
10	13	14	18	1	13	42	35	4	11	27	25	7	12	66	67	10	15	35	35	1	16	44	49	4	11	68	66	7	16	19	19				
10	14	33	33	1	14	56	53	4	13	22	17	7	13	13	11	10	18	15	15	1	17	40	44	4	13	28	26	7	17	12	15				
10	17	21	22	1	15	15	9	4	14	74	77	7	14	40	41	11	2	11	8	1	19	11	19	4	14	50	48	7	18	14	22				
10	18	23	23	1	16	45	47	4	15	61	63	7	16	18	18	11	3	17	17	1	20	44	43	4	15	56	60	7	19	18	18				
11	1	17	28	1	17	109	108	4	16	101	97	7	17	13	28	11	4	4	9	1	21	14	18	4	16	57	54	7	20	15	16				
11	2	18	8	1	18	38	44	4	18	56	59	7	19	12	16	11	5	15	16	1	23	15	13	4	17	27	27	7	21	15	18				
11	4	9	8	1	19	16	19	4	19	26	29	7	20	29	32	11	6	10	6	1	25	23	24	4	18	73	78	8	1	28	24				
11	5	11	12	1	22	13	18	4	20	31	32	7	21	25	26	11	7	15	16	2	1	69	64	4	22	21	23	8	2	15	16				
11	6	19	20	1	23	38	42	4	21	37	37	7	22	34	35	11	8	48	47	2	2	9	5	4	24	15	13	8	3	12	9				
11	7	13	12	1	25	20	20	4	24	33	34	8	1	18	18	11	9	42	39	2	3	59	58	5	1	120	112	8	4	108	99				
11	9	28	27	2	1	20	21	5	1	24	15	8	2	117	112	11	11	27	21	2	4	170	149	5	2	92	87	8	5	64	62				
11	10	28	28	2	2	59	50	5	2	6	5	8	3	22	22	11	12	21	22	2	5	37	41	5	3	95	85	8	6	75	72				
11	11	57	56	2	4	64	64	5	3	97	90	8	4	18	11	11	13	35	33	2	6	78	65	5	4	90	91	8	7	45	43				
11	14	14	15	2	5	24	19	5	4	22	17	8	5	15	7	11	15	18	18	2	7	72	77	5	5	15	10	8	8	38	36				
11	15	18	18	2	6	203	188	5	5	70	74	8	6	57	53	12	2	53	50	2	8	361	340	5	6	53	51	8	9	61	59				
12	1	27	23	2	8	35	38	5	6	62	55	8	7	30	30	12	3	10	6	2	9	15	19	5	7	81	77	8	11	78	75				
12	2	47	44	2	9	166	148	5	7	32	34	8	8	18	8	12	6	24	24	2	10	122	106	5	8	11	11	8	12	29	28				
12	4	41	40	2	10	247	251	5	8	32	28	8	9	58	57	12	7	17	21	2	11	129	124	5	9	52	44	8	14	27	29				
12	5	12	6	2	12	7	10	5	9	79	75	8	10	8	8	12	8	11	6	2	12	117	119	5	10	52	50	8	15	19	16				
12	9	20	22	2	13	44	45	5	10	44	44	8	12	8	6	12	11	21	19	2	13	33	31	5	11	32	35	8	16	27	26				
12	10	21	22	2	15	39	42	5	12	19	20	8	13	56	55	12	12	29	30	2	14	44	51	5	12	95	90	8	17	30	30				
12	13	13	12	2	16	72	72	5	14	95	91	8	14	28	28	12	13	14	13																

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
8	20	11	17	M = -1				3	7	18	15	6	12	24	27	10	2	24	23	1	22	36	40	5	13	42	40	8	12	52	51
9	1	54	46					3	8	167	163	6	13	64	63	10	4	56	56	1	25	20	31	5	14	14	18	8	13	28	27
9	2	67	63	0	4	242	215	3	9	183	174	6	14	30	25	10	5	38	24	2	1	25	6	5	15	59	55	8	14	48	58
9	3	90	84					3	12	73	75	6	15	30	30	10	6	49	49	2	2	27	46	5	16	18	15	8	15	26	26
9	4	60	56	0	6	80	60	3	15	52	57	6	16	24	23	10	7	16	16	2	3	129	97	5	17	24	27	8	18	18	17
9	5	10	6	0	8	95	95	3	17	29	47	6	17	23	24	10	9	10	12	2	4	124	91	5	19	30	31	9	1	19	19
9	6	17	10	0	10	108	91	3	21	33	35	6	18	12	12	10	12	16	15	2	5	89	91	5	21	21	25	9	2	108	106
9	7	16	13	0	12	109	98	3	23	15	23	6	20	36	39	10	13	22	24	2	6	212	201	5	22	22	28	9	3	52	51
9	10	10	7	0	14	79	77	3	25	12	11	7	1	58	58	10	14	23	23	2	8	165	151	5	24	12	15	9	4	48	47
9	12	41	40	0	16	138	130	4	1	70	63	7	2	66	64	10	15	29	27	2	10	139	130	6	0	113	110	9	5	46	46
9	13	20	20	0	18	42	37	4	2	215	200	7	3	36	31	10	16	10	11	2	12	47	45	6	1	46	48	9	6	28	22
9	14	17	14	0	20	19	22	4	3	34	22	7	4	41	39	10	18	14	10	2	14	20	21	6	2	10	5	9	7	33	29
9	15	26	29	0	24	15	15	4	4	48	43	7	5	26	23	11	1	19	20	2	18	37	39	6	3	50	53	9	9	10	8
9	16	49	46	1	1	157	189	4	5	44	41	7	6	100	92	11	2	19	19	2	22	30	51	6	4	100	100	9	10	13	14
9	17	16	20	1	2	93	96	4	6	39	40	7	7	95	93	11	3	40	38	3	1	36	8	6	5	56	55	9	11	52	51
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10	2	40	38	1	4	146	141	4	8	113	113	7	9	79	77	11	5	15	14	3	3	123	121	6	7	68	61	9	14	17	18
10	3	53	55	1	5	13	57	4	9	124	112	7	10	38	35	11	6	14	14	3	4	148	150	6	8	95	96	9	15	35	38
10	5	10	15	1	6	139	110	4	10	51	49	7	12	80	61	11	7	17	17	3	5	124	112	6	9	52	51	9	16	16	13
10	6	35	34	1	7	67	66	4	11	50	47	7	13	29	20	11	8	43	43	3	6	75	71	6	10	74	67	9	17	21	23
10	8	60	58	1	8	48	39	4	12	28	31	7	17	10	12	11	9	9	11	3	7	152	148	6	11	12	14	10	0	32	31
10	9	10	6	1	9	184	176	4	13	50	48	7	18	17	16	11	11	35	33	3	8	58	48	6	12	14	18	10	1	53	54
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10	14	21	21	1	13	104	95	4	25	16	15	8	2	102	99	12	1	15	14	3	12	73	67	6	17	26	28	10	5	19	14
10	15	16	16	1	14	45	43	5	1	86	77	8	3	57	60	12	2	27	28	3	16	47	56	6	18	26	24	10	8	39	39
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11	3	33	32	1	17	35	34	5	3	16	15	8	5	20	20	12	7	33	33	3	25	14	13	6	22	25	29	10	11	17	19
11	4	12	13	1	18	35	36	5	4	11	16	8	6	31	30	12	10	28	26	4	0	215	221	6	23	14	17	10	12	12	16
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11	7	10	9	1	25	28	22	5	7	10	10	8	9	59	55	13	3	23	20	4	3	95	73	7	5	77	77	10	17	10	8
11	9	16	9	2	1	46	21	5	8	58	68	8	10	33	34	13	4	16	19	4	4	115	107	7	6	63	61	11	1	35	35
11	10	34	35	2	2	92	104	5	9	120	126	8	11	38	42	13	5	34	31	4	5	67	66	7	7	131	130	11	4	31	32
11	11	19	18	2	3	41	47	5	10	19	22	8	12	46	44	13	7	14	11	4	6	66	68	7	8	112	108	11	5	43	45
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11	13	42	39	2	5	177	135	5	12	18	20	8	14	34	38	13	10	28	26	4	9	72	74	7	11	33	34	11	7	16	18
12	1	16	13	2	6	320	266	5	13	67	63	8	16	45	46	13	11	16	15	4	10	45	41	7	12	67	65	11	8	31	29
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12	4	37	36	2	9	168	148	5	17	38	43	9	2	54	55	13	14	107	107	4	14	107	107	7	15	40	38	11	11	9	6
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12	10	19	18	2	18	9	14	6	2	75	75	9	8	17	15	13	19	16	14	5	2	69	61	8	0	84	89	12	5	21	25
12	11	14	12	2	20	31	35	6	3	38	38	9	10	30	30	13	20	18	21	5	3	62	54	8	2	36	40	12	6	27	27
12	12	32	31	2	21	13	27	6	4	11	12	9	11	18	18	1	3	23	16	5	4	106	95	8	3	54	48	12	9	16	14
13	1	30	29	2	24	25	27	6	5	61	61	9	12	15	13	1	4	20	13	5	5	28	28	8	4	19	17	12	11	12	12
13	2	31	31	3	1	63	57	6	6	127	122	9	13	36	40	1	5	39	30	5	6	43	42	8	5	56	53	12	12	19	19
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13	4	10	10	3	3	121	112	6	8	94	94	9	16	17	15	1	7	127	119	5	8	58	55	8	7	10	9	13	2	15	17
13	7	20	17	3	4	111	103	6	9	35	31	9	17	15	15	1	8	14	43	5	9	80	69	8	8	52	49	13	3	21	20
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Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
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0	4	63	50	3	7	13	12	6	3	17	6	9	8	13	13	0	24	25	20	3	21	40	43	6	20	18	20	10	7	12	10
				3	8	44	37	6	4	41	36	9	10	21	25	1	0	114	154	4	0	96	111	6	21	25	24	10	9	33	34
				3	9	66	66	6	5	44	39	9	11	12	12	1	1	121	134	4	1	10	10	7	0	10	12	10	10	25	23
0	6	18	14	3	10	87	77	6	6	139	136	9	12	14	16	1	2	148	140	4	2	66	66	7	1	12	9	10	11	24	22
0	8	21	23	3	11	47	40	6	7	31	33	9	13	30	31	1	3	93	105	4	3	39	37	7	2	24	24	10	13	41	41
0	10	95	98	3	12	40	38	6	8	129	125	9	14	25	24	1	4	44	34	4	4	52	83	7	3	68	73	10	16	19	19
0	12	183	180	3	13	49	48	6	9	33	28	9	15	34	36	1	5	44	37	4	5	20	10	7	4	44	46	11	3	28	30
0	14	88	83	3	14	48	47	6	10	8	11	9	16	18	20	1	6	29	24	4	6	35	30	7	5	11	10	11	4	22	18
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0	18	27	27	3	17	43	64	6	13	34	32	10	1	45	51	1	8	61	54	4	8	30	26	7	7	106	101	11	8	13	8
0	20	51	50	3	18	62	66	6	14	9	7	10	2	47	40	1	9	59	52	4	10	118	115	7	9	67	68	11	9	15	19
0	22	38	39	3	19	31	40	6	15	35	36	10	3	30	32	1	10	13	32	4	11	24	25	7	10	32	24	11	13	12	13
0	24	12	14	3	21	42	50	6	17	24	25	10	4	34	35	1	11	207	199	4	12	50	52	7	11	49	45	11	14	20	23
1	0	126	144	4	0	87	80	6	19	26	20	10	5	28	20	1	12	67	67	4	13	38	33	7	12	9	7	12	0	30	40
1	2	36	35	4	1	10	3	6	20	49	50	10	6	63	62	1	15	49	47	4	14	47	49	7	13	12	9	12	2	12	15
1	3	71	51	4	2	115	112	6	22	14	15	10	8	41	41	1	16	26	32	4	15	30	26	7	14	36	39	12	4	13	14
1	4	182	184	4	3	49	44	7	1	21	23	10	10	10	9	1	17	68	71	4	16	18	15	7	16	44	45	12	5	23	23
1	5	66	55	4	4	45	37	7	2	42	40	10	11	36	34	1	19	44	45	4	17	9	10	7	17	12	11	12	6	12	15
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1	9	16	17	4	8	33	30	7	6	60	57	11	1	15	17	2	2	161	171	5	0	72	74	7	21	19	21				
1	10	45	44	4	9	20	21	7	7	12	13	11	2	27	25	2	3	92	97	5	1	45	43	8	0	73	82				
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1	15	17	24	4	13	54	50	7	11	12	14	11	6	38	39	2	6	26	20	5	5	48	39	8	5	13	13				
1	17	43	40	4	14	13	9	7	12	14	16	11	8	11	11	2	9	43	43	5	6	58	45	8	6	41	42				
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2	0	34	79	4	17	27	34	7	15	14	16	12	0	9	7	2	13	68	67	5	9	8	5	8	9	22	24				
2	1	44	21	4	18	26	26	7	16	25	23	12	1	26	28	2	15	27	25	5	10	49	49	8	10	11	14				
2	2	54	33	4	19	29	33	7	18	52	51	12	4	19	20	2	16	51	55	5	11	71	73	8	11	9	5				
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2	4	77	76	4	23	15	17	8	1	14	19	12	7	21	22	2	20	29	32	5	14	21	23	8	14	41	41				
2	5	124	131	5	0	127	134	8	2	58	63	12	12	22	22	2	21	17	23	5	17	21	21	8	15	42	39				
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2	8	166	158	5	2	39	28	8	4	15	15	13	1	13	12	3	0	13	34	5	19	34	37	8	19	24	24				
2	9	21	16	5	3	40	48	8	5	26	25	13	2	16	14	3	1	30	18	5	21	20	21	9	0	42	41				
2	10	60	50	5	4	88	91	8	6	53	55	13	3	29	31	3	3	170	171	5	22	21	22	9	1	19	18				
2	11	10	15	5	5	75	71	8	7	32	25	13	4	9	6	3	4	61	69	6	0	16	18	9	2	51	51				
2	12	20	26	5	6	22	14	8	8	34	34	13	5	79	78	3	5	79	78	6	1	43	47	9	4	32	33				
2	13	14	19	5	7	25	27	8	9	26	30	13	6	51	50	3	6	51	50	6	2	7	6	9	5	16	17				
2	14	61	60	5	8	76	70	8	10	28	25	13	7	113	105	3	7	113	105	6	3	16	17	9	7	41	41				
2	15	35	38	5	10	42	45	8	12	57	60	0	0	165	207	3	8	10	13	6	4	150	151	9	8	42	46				
2	16	45	49	5	12	78	74	8	13	33	35	0	2	167	209	3	9	19	17	6	5	24	30	9	9	18	18				
2	17	44	46	5	13	42	43	8	15	13	12	3	10	9	19	3	10	9	19	6	6	158	159	9	11	21	19				
2	20	78	85	5	15	23	21	8	16	39	42	0	4	53	65	3	11	115	104	6	7	67	62	9	12	45	44				
2	23	16	19	5	16	9	8	8	17	37	37	0	6	25	21	3	12	19	21	6	9	57	56	9	13	32	30				
3	0	102	87	5	17	34	34	8	18	18	17	0	8	47	49	3	13	19	20	6	10	32	31	9	14	31	30				
3	1	133	124	5	18	13	17	8	19	28	27	0	10	146	147	3	14	64	61	6	12	29	26	9	17	15	16				
3	2	13	1	5	19	20	26	9	0	105	109	0	12	90	84	3	16	37	35	6	13	12	18	10	1	33	32				
3	3	31	15	5	21	21	23	9	1	49	49	0	14	111	109	3	17	67	72	6	15	33	33	10	2	24	22				
3	4	110	98	6	0	11	7	9	4	65	64	0	16	8	7	3	18	41	47	6	16	18	14	10	4	33	30				
3	5	106	94	6	1	8	9	9	5	40	43	0	18	60	58	3	14	51	56	6	18	57	57	10	5	9	10				

M= 3

0 0 172 182

0 2 244 248

0 4 25 29

0 6 107 99

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
2	3	72	69	5	3	57	54	8	4	16	20	13	6	97	95	6	7	82	80	10	7	34	39	1	28	16	17	1	28	16	17
2	4	86	86	5	5	91	90	8	5	63	60					6	8	44	48	10	8	42	39	1	21	18	20	1	21	18	20
2	5	45	42	5	6	94	91	8	6	26	24	M*	4			6	9	24	24	10	9	25	22	2	8	113	146	2	8	113	146
2	6	76	87	5	7	60	49	8	7	20	21					6	10	11	29	10	10	10	9	2	1	86	91	2	1	86	91
2	7	68	59	5	8	66	59	8	8	35	36	8	8	48	52	6	11	76	73	6	11	28	31	2	2	114	126	2	2	114	126
2	8	37	38	5	9	83	85	8	11	32	33	0	4	154	170	3	13	25	21	6	13	34	33	10	12	12	9	2	3	27	33
2	10	105	104	5	10	134	129	8	12	36	39	0	6	31	24	3	14	44	43	6	14	15	15	10	13	25	26	2	4	194	188
2	11	62	61	5	11	40	40	8	13	11	13	0	8	86	87	3	15	10	10	6	15	9	6	10	14	20	17	2	5	44	48
2	12	113	104	5	12	11	7	8	14	27	26	0	10	247	245	3	17	26	24	6	16	13	14	11	0	36	41	2	6	16	18
2	14	64	66	5	13	43	44	8	15	10	21	0	12	52	51	3	18	47	46	6	18	45	43	11	1	14	17	2	7	9	8
2	15	30	33	5	14	48	47	8	16	12	7	0	14	62	59	3	19	11	13	6	20	22	23	11	2	15	17	2	9	14	15
2	16	58	60	5	15	10	10	8	17	32	31	0	16	24	26	3	22	19	21	7	0	109	124	11	3	32	31	2	10	9	12
2	18	44	45	5	16	15	15	9	0	21	21	0	18	37	37	4	0	9	11	7	1	16	14	11	4	19	21	2	11	16	16
2	20	29	31	5	17	30	30	9	1	26	24	0	22	31	31	4	1	112	121	7	2	75	81	11	5	32	32	2	12	17	28
2	22	17	28	5	19	36	35	9	2	22	18	1	0	11	6	4	2	85	87	7	3	98	100	11	6	16	19	2	13	21	19
3	0	62	65	6	0	10	12	9	3	8	8	1	1	151	170	4	3	38	36	7	4	63	65	11	9	25	28	2	16	45	41
3	1	102	103	6	1	45	43	9	4	50	50	1	2	42	46	4	4	107	113	7	5	42	46	12	0	14	10	2	18	18	20
3	2	117	120	6	2	54	95	9	5	33	37	1	3	213	210	4	5	116	119	7	6	87	85	12	1	28	26	2	20	20	19
3	3	78	71	6	3	28	31	9	6	44	44	1	4	55	45	4	6	105	106	7	11	40	38	12	2	22	22	3	0	19	25
3	4	88	94	6	4	133	139	9	7	24	27	1	5	86	78	4	7	76	81	7	12	21	17	12	5	29	30	3	1	201	220
3	5	91	91	6	5	81	77	9	8	15	17	1	6	42	34	4	8	14	12	7	13	15	14	12	8	28	25	3	2	229	231
3	6	68	69	6	6	55	55	9	9	13	13	1	7	21	15	4	10	136	139	7	14	38	35	13	1	20	24	3	4	23	37
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3	10	15	18	6	10	50	48	9	14	24	25	1	11	163	161	4	15	20	24	8	0	22	23					3	9	36	42
3	11	46	44	6	11	46	44	9	15	12	14	1	12	64	61	4	16	38	36	8	1	82	88					3	10	23	27
3	12	52	49	6	14	14	7	9	17	21	20	1	13	73	70	4	17	22	23	8	2	16	16					3	11	50	49
3	13	79	76	6	15	23	23	10	2	10	10	1	14	16	16	4	18	13	16	8	5	47	50					3	12	22	20
3	14	11	13	6	16	32	35	10	4	24	21	1	16	16	17	4	19	12	13	8	6	26	27					3	14	10	4
3	15	47	47	6	17	24	26	10	4	55	54	1	17	37	33	4	22	10	12	8	7	58	47					3	15	12	18
3	16	53	53	6	18	22	24	10	5	30	29	1	18	11	11	5	0	11	12	8	8	49	42					3	16	32	38
3	17	36	35	6	19	11	9	10	6	12	5	1	23	15	14	5	1	89	92	8	9	18	16					3	21	10	12
3	18	21	25	6	20	32	33	10	7	9	5	2	0	129	150	5	2	63	64	8	10	46	50					4	0	24	29
3	19	44	46	7	0	55	59	10	8	49	47	2	1	49	58	5	3	96	102	8	11	19	18					4	1	79	78
3	20	24	24	7	1	12	13	10	9	43	43	2	2	193	204	5	4	21	26	8	12	16	15					4	2	182	110
4	0	66	76	7	2	67	69	10	10	11	12	2	3	51	60	5	5	73	74	8	13	25	24					4	3	121	131
4	1	66	69	7	3	11	14	10	11	43	39	2	4	145	149	5	6	114	114	8	15	21	19					4	4	44	35
4	2	39	45	7	4	78	82	10	12	12	11	2	5	24	24	5	7	12	14	8	18	27	27					4	5	15	12
4	3	48	47	7	5	109	112	10	15	15	15	2	6	58	57	5	8	112	110	9	0	19	27					4	6	32	31
4	4	79	72	7	6	12	17	11	2	26	28	2	7	18	17	5	9	64	61	9	1	13	15					4	7	22	22
4	5	18	15	7	7	60	85	11	4	19	25	2	8	11	14	5	10	19	19	9	2	38	43					4	8	79	82
4	6	48	58	7	8	45	45	11	5	44	43	2	9	21	22	5	11	67	62	9	3	21	17					4	10	42	43
4	7	26	33	7	9	63	63	11	6	15	13	2	10	107	102	5	12	76	77	9	5	25	29					4	12	45	44
4	8	122	118	7	10	14	14	11	7	32	33	2	12	11	11	5	13	25	32	9	6	43	48					4	14	44	45
4	9	51	54	7	12	18	20	11	10	14	17	2	13	39	36	5	15	27	38	9	8	53	55					4	15	14	14
4	10	23	16	7	13	16	16	11	12	24	23	2	16	24	25	5	16	14	14	9	10	19	19					4	16	27	29
4	11	46	46	7	16	48	47	11	13	13	13	2	18	28	28	5	17	20	20	9	11	21	22					4	18	13	18
4	12	124	118	7	17	24	23	12	0	37	43	2	20	26	26	5	19	10	9	9	12	43	41					4	21	12	18
4	13	16	16	7	18	27	29	12	1	15	16	2	22	18	19	6	0	45	50	9	13	12	13					5	0	43	45
4	17	47	45	7	19	38	39	12	3	28	27	3	0	95	123	6	1	74	76	9	15	13	11					5	1	96	101
4	20	18	20	7	20	15	16	12	5	12	10	3	1	45	44	6	2	65	77	10	1	31	28					5	2	52	55
4	21	12	13	8	0	46	50	12	7	16	17	3	2	88	90	6	3	26	26	10	3	11	14					5	3	27	35
5	0	25	24	8	1	11	12	12	8	13	12	3	3	186	196	6	4	81	83	10	4	17	12					5	4	96	95
5	1	22	20	8	2	8	4	13	0	21	22	3	4	176	169	6	5	58	57	10	5	26	28					5	5	57	58
5	2	96	96	8	3	70	71	13	1	25	26	3	5	115	105	6	6	105	100	10	6	45	45					5	6	47	48

Table A. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
5	7	17	19	8	16	23	23	1	3	102	108	4	10	63	57	8	1	25	24	1	2	45	54	4	9	44	42	8	8	48	45
5	8	50	48	9	2	31	34	1	4	38	50	4	11	26	24	8	2	11	12	1	3	68	77	4	10	15	17	8	9	26	25
5	9	71	66	9	4	39	41	1	5	59	70	4	12	34	33	8	3	21	26	1	5	82	80	4	11	13	15	8	10	39	38
5	10	56	53	9	6	25	25	1	6	27	29	4	14	42	40	8	4	16	14	1	6	54	58	4	12	40	41	8	13	37	37
5	11	52	50	9	8	35	33	1	7	29	30	4	15	11	11	8	5	10	12	1	7	17	17	4	13	30	30	8	14	16	14
5	12	39	34	9	9	37	37	1	8	43	45	4	16	22	22	8	6	52	55	1	8	24	25	4	14	10	12	8	15	15	16
5	13	12	12	9	10	39	38	1	9	12	9	4	17	20	21	8	10	51	54	1	9	34	37	4	15	13	17	9	1	37	37
5	14	15	16	9	11	27	26	1	10	27	24	4	18	11	11	8	11	23	22	1	10	14	12	4	16	44	43	9	2	24	27
5	16	25	26	9	12	17	16	1	11	32	33	4	19	17	17	8	12	23	23	1	11	19	19	4	18	23	23	9	4	9	7
5	17	23	25	9	14	10	7	1	12	20	21	4	20	28	27	8	13	10	9	1	12	29	30	4	19	15	13	9	5	15	18
5	20	30	30	9	15	15	13	1	13	14	21	5	8	19	16	9	0	21	25	1	13	63	57	5	1	62	65	9	6	22	22
6	0	48	51	9	16	16	16	1	14	39	38	5	1	19	20	9	1	21	23	1	15	62	57	5	2	12	20	9	7	31	31
6	1	64	70	10	0	14	15	1	15	60	60	5	2	15	12	9	3	30	27	1	16	19	19	5	3	24	34	9	8	10	6
6	2	57	63	10	1	16	14	1	17	20	21	5	3	83	91	9	5	13	11	1	17	14	16	5	4	31	29	9	11	26	25
6	3	74	80	10	2	15	10	1	18	13	17	5	6	34	28	9	6	10	19	1	18	18	8	5	5	22	20	10	0	30	36
6	4	133	139	10	3	12	12	1	21	33	34	5	7	65	66	9	7	38	40	1	19	12	9	5	6	51	49	10	2	10	9
6	5	36	36	10	4	17	17	2	0	44	47	5	8	24	22	9	8	20	18	1	20	20	20	5	7	33	32	10	4	25	28
6	6	34	31	10	5	28	26	2	1	53	48	5	9	46	46	9	9	33	33	2	0	137	153	5	8	38	37	10	5	11	10
6	7	20	21	10	6	46	45	2	2	205	229	5	11	8	10	9	10	24	24	2	2	34	37	5	9	31	29	10	6	23	23
6	8	24	26	10	9	32	35	2	3	49	46	5	12	10	10	9	11	14	15	2	3	91	92	5	13	27	26	10	7	9	10
6	9	25	31	10	10	27	25	2	4	96	98	5	14	27	26	9	14	19	15	2	4	38	39	5	14	44	42	10	8	17	16
6	10	38	36	10	13	14	11	2	5	40	30	5	15	26	28	10	0	35	38	2	5	10	12	5	15	30	31	11	1	42	44
6	11	28	29	10	14	18	19	2	6	87	86	5	16	30	27	10	1	17	19	2	6	86	93	5	16	26	25	11	2	23	22
6	13	16	16	11	1	22	22	2	7	8	9	5	17	23	24	10	2	21	26	2	7	13	18	5	17	11	7	11	3	25	26
6	16	35	35	11	2	23	26	2	8	47	49	5	18	47	47	10	3	17	17	2	8	20	19	5	18	22	24	11	4	20	20
6	17	11	13	11	4	20	22	2	10	13	12	6	0	13	34	10	7	13	15	2	9	24	24	6	0	62	72	12	2	18	19
6	18	31	31	11	6	14	14	2	12	15	22	6	1	22	22	10	8	31	31	2	10	62	62	6	1	9	7	12	3	16	18
7	0	9	15	11	7	26	25	2	13	24	26	6	2	92	102	10	10	21	19	2	12	56	53	6	4	53	54				
7	1	42	37	11	9	26	26	2	14	77	72	6	3	11	9	10	11	12	12	2	13	24	23	6	5	32	39				
7	2	123	134	12	0	45	47	3	0	113	123	6	4	20	18	10	12	14	11	2	14	39	39	6	6	58	57				
7	3	41	40	12	1	13	11	3	1	83	91	6	5	11	16	11	0	28	32	2	16	44	43	6	7	54	55				
7	4	46	51	12	2	14	12	3	2	93	105	6	6	14	16	11	2	16	19	2	19	11	11	6	8	46	46				
7	5	45	42	12	3	38	28	3	3	93	86	6	7	12	16	11	3	29	27	2	20	17	19	6	9	20	20				
7	6	32	32	12	4	12	11	3	4	82	76	6	8	61	66	11	4	22	20	3	0	30	37	6	12	18	19				
7	7	8	10	12	6	20	19	3	5	56	55	6	9	37	40	11	5	17	17	3	1	122	132	6	13	25	24				
7	8	34	29	12	8	24	26	3	6	25	33	6	10	29	29	11	7	22	24	3	2	29	31	6	14	21	20				
7	9	79	80	13	1	12	12	3	7	12	12	6	13	18	18	12	0	31	35	3	3	47	51	6	15	28	28				
7	10	11	10	13	2	12	9	3	8	45	47	6	14	19	22	12	1	25	26	3	4	42	41	6	16	14	14				
7	11	15	13	13	3	12	10	3	9	19	21	6	15	28	28	12	2	14	10	3	5	38	40	7	0	12	13				
7	12	18	20					3	10	37	34	6	17	26	26	12	5	16	17	3	6	27	26	7	1	51	53				
7	14	11	8					3	11	21	21	7	0	85	95	12	6	22	21	3	8	68	67	7	2	36	34				
7	15	25	26					3	12	38	39	7	1	14	11					3	9	68	71	7	3	34	36				
7	16	11	12					3	13	27	27	7	3	45	44					3	10	34	33	7	4	23	24				
8	0	68	70					3	14	26	25	7	4	61	62					3	11	14	10	7	5	20	23				
8	1	52	60					3	15	34	34	7	5	28	31					3	12	54	54	7	6	15	16				
8	3	59	64					3	16	14	16	7	6	13	12					3	13	20	21	7	8	62	62				
8	4	10	12					3	21	31	31	7	7	49	52					3	14	22	25	7	9	24	21				
8	5	17	20					4	0	23	25	7	8	15	12					3	15	36	37	7	10	11	11				
8	6	37	34					4	1	13	21	7	9	20	23					3	16	23	23	7	12	42	39				
8	7	16	18					4	2	13	23	7	10	44	45					3	17	19	18	7	14	36	34				
8	8	55	59					4	3	52	55	7	12	22	24					3	19	16	17	7	15	24	25				
8	9	24	27					4	4	30	31	7	13	10	11					4	0	15	14	8	0	14	19				
8	11	10	12					4	5	15	17	7	14	10	12					4	2	38	42	8	2	20	23				
8	12	28	26					4	6	45	43	7	16	11	14					4	4	14	16	8	3	14	9				
8	13	15	11					4	7	24	24	7	17	29	29					1	0	15	28	8	4	27	26				
8	14	11	10					4	8	8	4	8	0	32	34					1	1	79	94	4	8	62	80				

Table A. (continued)

K	L	FD	FC	K	L	FD	FC	K	L	FD	FC	K	L	FD	FC	K	L	FD	FC	K	L	FD	FC	K	L	FD	FC	K	L	FD	FC	K	L	FD	FC
2	14	52	51	6	14	27	26	0	6	41	38	4	12	44	41	9	7	19	18	3	14	13	14	9	1	9	6	3	14	28	19	3	14	28	19
2	16	30	30	6	15	14	14	0	8	74	73	4	13	17	17	9	8	10	6	3	15	12	10	9	2	43	43	3	15	16	14	3	15	16	14
3	0	26	28	6	16	14	16	0	10	8	15	4	14	11	7	9	9	24	21	3	16	21	19	9	3	18	18	4	0	18	19	4	0	18	19
3	1	37	40	7	1	23	25	0	12	67	68	4	16	20	20	10	0	41	43	4	0	69	71	9	4	23	21	4	1	12	14	4	1	12	14
3	2	30	38	7	2	9	6	0	14	26	27	5	0	61	68	10	1	26	29	4	1	36	37	9	5	23	20	4	2	16	18	4	2	16	18
3	3	24	26	7	4	32	36	0	16	16	17	5	1	26	24	10	2	41	43	4	2	40	45	9	6	17	14	4	3	27	38	4	3	27	38
3	4	29	28	7	5	11	10	1	0	47	55	5	2	42	45	10	4	10	9	4	3	35	39	9	7	9	9	4	4	50	54	4	4	50	54
3	5	33	40	7	6	37	34	1	1	79	86	5	3	28	26	10	5	22	22	4	4	45	47	9	8	10	10	4	5	15	14	4	5	15	14
3	6	63	71	7	7	38	39	1	2	65	64	5	4	34	36	10	6	17	16	4	5	9	15	10	0	35	39	4	6	39	48	4	6	39	48
3	7	89	86	7	8	10	28	1	3	50	57	5	5	41	41	10	7	20	20	4	6	64	67	10	1	16	15	4	8	11	7	4	8	11	7
3	9	22	23	7	10	56	56	1	4	64	68	5	6	57	61	11	3	36	38	4	7	10	20	10	3	21	20	4	10	11	11	4	10	11	11
3	10	78	74	7	11	17	18	1	5	70	71	5	7	55	57	11	4	10	7	4	8	28	29	10	4	31	33	4	11	14	13	4	11	14	13
3	12	16	18	7	12	13	14	1	6	43	41	5	8	10	10	4	9	14	10	4	9	14	10	10	6	8	7	4	12	25	23	4	12	25	23
3	13	43	43	7	13	21	23	1	7	44	48	5	10	14	17	4	10	26	26	4	10	26	26	11	0	9	12	4	13	9	11	4	13	9	11
3	14	37	36	7	14	28	27	1	8	31	29	5	11	23	23	4	13	10	12	4	13	10	12	11	1	27	27	4	14	9	4	4	14	9	4
3	15	12	12	8	0	32	37	1	9	36	36	5	14	13	14	0	0	144	155	4	14	13	14	11	3	26	27	5	0	29	31	5	0	29	31
3	17	18	17	8	3	23	22	1	11	45	44	5	15	14	13	0	2	47	56	5	1	16	16	5	1	16	16	5	1	7	6	5	1	7	6
4	0	62	70	8	4	9	5	1	12	15	11	6	0	46	52	0	4	88	88	5	8	31	31	5	8	31	31	5	2	10	13	5	2	10	13
4	2	21	16	8	5	28	26	1	15	28	27	6	1	43	48	0	6	56	56	5	9	11	14	5	9	11	14	5	3	30	32	5	3	30	32
4	3	24	27	8	6	38	37	1	16	12	14	6	2	21	24	0	8	43	39	5	10	25	22	8	0	50	54	5	4	53	52	5	4	53	52
4	4	12	18	8	8	22	22	1	18	11	8	6	3	12	12	0	10	17	11	5	11	15	13	0	2	81	82	5	5	14	16	5	5	14	16
4	5	45	48	8	9	26	28	2	0	98	107	6	4	27	29	0	12	25	26	5	13	10	11	0	4	24	29	5	6	11	13	5	6	11	13
4	6	87	83	8	10	12	12	2	1	18	12	6	5	49	52	0	14	24	21	5	14	9	11	0	6	30	29	5	7	25	24	5	7	25	24
4	7	14	14	8	11	37	39	2	2	8	5	6	6	29	29	1	0	15	17	6	0	10	8	0	8	26	26	5	8	32	32	5	8	32	32
4	8	18	18	8	12	32	30	2	3	9	15	6	7	33	33	1	1	21	20	6	1	25	28	0	12	37	34	5	9	21	20	5	9	21	20
4	9	46	44	8	14	14	15	2	4	73	75	6	8	35	33	1	2	64	68	6	3	51	56	0	14	8	6	5	10	13	9	5	10	13	9
4	11	22	26	9	0	20	21	2	5	32	32	6	9	12	13	1	4	22	12	6	4	29	29	1	0	85	90	5	11	12	15	5	11	12	15
4	14	53	53	9	1	10	8	2	6	53	53	6	10	15	15	1	5	60	59	6	5	8	5	1	1	30	31	5	12	26	23	5	12	26	23
4	15	24	22	9	2	30	34	2	7	19	19	6	11	14	12	1	6	52	50	6	6	45	42	1	2	16	15	6	0	15	16	6	0	15	16
4	17	11	11	9	4	42	45	2	8	68	67	6	12	24	23	1	9	13	12	6	7	35	34	1	3	10	9	6	1	12	12	6	1	12	12
4	18	15	15	9	5	15	14	2	9	27	27	6	14	24	23	1	10	16	15	6	8	12	12	1	4	44	41	6	2	24	23	6	2	24	23
5	0	54	50	9	8	17	16	2	10	50	49	7	0	18	22	1	11	34	32	6	9	8	8	1	6	23	26	6	3	25	21	6	3	25	21
5	2	37	48	9	9	28	20	2	12	27	25	7	1	17	21	1	14	13	14	6	10	9	6	1	8	24	24	6	4	45	46	6	4	45	46
5	4	58	58	9	10	13	14	2	14	51	48	7	2	19	23	1	16	10	11	6	11	18	16	1	9	24	24	6	5	28	28	6	5	28	28
5	5	25	24	9	11	28	27	3	0	14	18	7	3	18	20	1	17	19	16	6	12	26	26	1	10	13	12	6	6	11	16	6	6	11	16
5	6	10	15	9	12	28	21	3	1	44	51	7	5	36	35	2	0	43	53	7	0	20	18	1	11	29	27	6	7	12	13	6	7	12	13
5	7	47	47	10	1	17	14	3	2	13	18	7	6	45	45	2	1	29	31	7	1	26	28	1	12	19	17	6	9	17	17	6	9	17	17
5	8	35	34	10	2	49	51	3	3	48	53	7	8	37	35	2	3	24	29	7	2	22	26	1	14	13	13	6	10	16	15	6	10	16	15
5	9	18	39	10	3	26	26	3	5	70	63	7	10	19	19	2	5	14	14	7	3	23	23	1	15	24	21	6	11	15	16	6	11	15	16
5	10	18	18	10	4	29	30	3	6	34	36	7	11	17	15	2	6	90	95	7	4	39	39	2	0	72	71	7	0	9	12	7	0	9	12
5	11	12	11	10	5	15	16	3	7	66	66	7	12	34	32	2	8	20	22	7	5	17	13	2	1	7	8	7	1	8	6	7	1	8	6
5	12	20	18	10	7	12	9	3	8	70	65	8	1	20	25	2	12	38	36	7	7	17	15	2	2	41	42	7	5	25	24	7	5	25	24
5	13	39	37	10	9	18	11	3	9	24	21	8	4	16	19	3	0	44	49	7	8	27	27	2	3	8	7	7	6	9	10	7	6	9	10
5	15	11	15	11	0	19	20	3	11	13	12	8	5	16	15	3	1	17	9	7	10	18	16	2	4	52	54	7	10	11	11	7	10	11	11
5	16	32	33	11	1	30	32	3	12	40	41	8	6	14	15	3	2	14	15	7	12	11	12	2	5	7	9	7	11	16	16	7	11	16	16
6	0	13	16	11	3	12	11	3	15	29	29	8	7	29	29	3	3	25	25	7	13	19	15	2	7	18	20	8	2	13	13	8	2	13	13
6	2	59	62	11	5	19	19	3	16	19	17	8	9	12	14	3	4	20	18	8	0	8	14	2	10	22	21	8	4	28	28	8	4	28	28
6	3	43	44	11	6	23	23	4	0	20	19	8	10	29	28	3	5	88	93	8	1	22	23	2	11	15	15	8	6	20	20	8	6	20	20
6	4	46	48	12	0	13	18	4	1	30	34	8	11	19	19	3	6	24	24	8	3	21	21	2	12	9	10	8	8	14	15	8	8	14	15
6	5	36	35	12	1	13	16	4	2	30	33	8	12	22	23	3	7	22	25	8	5	14	14	2	13	12	12	9	0	33	33	9	0	33	33
6	6	34	39	12	2	15	16	4																											

Table A. (concluded)

K	L	FD	FC	K	L	FC	FC	K	L	FC	FC	K	L	FO	FC	K	L	FC	FC	K	L	FC	FC
10	3	8	5	5	4	8	11	2	1	13	17	1	3	29	27	1	6	12	10	H= 18			
10	4	22	24	5	5	19	16	2	2	36	35	1	5	12	12	1	7	9	12	1	6	12	6
H= 12				5	6	11	13	2	3	10	9	1	8	19	15	2	8	62	52				
				5	7	11	9	2	4	20	25	1	9	35	30	2	1	19	16				
				5	8	26	24	2	6	24	24	2	0	24	24	2	4	33	30				
0	0	45	54	5	9	16	14	2	8	24	22	2	2	54	49	2	6	24	22				
0	2	32	33	5	10	21	16	2	9	14	12	2	3	16	15	3	1	25	24				
0	4	8	6	5	12	26	24	2	10	23	19	2	4	22	21	3	2	36	35				
0	10	65	61	6	0	22	22	2	11	13	11	2	5	9	9	3	3	23	18				
0	14	13	11	6	1	13	9	3	0	20	17	2	8	34	31	3	4	14	11				
1	1	8	10	6	2	20	29	3	1	67	60	2	14	11	8	3	5	21	15				
1	2	45	43	6	4	14	15	3	2	14	16	3	0	30	27	3	6	20	16				
1	3	46	46	6	5	8	7	3	4	23	20	3	1	20	20	3	7	27	23				
1	4	13	14	6	6	21	20	3	7	32	34	3	2	10	10	4	0	21	15				
1	5	7	7	6	7	11	11	3	8	24	22	3	3	27	26	4	1	29	30				
1	8	25	26	6	8	13	11	3	11	23	19	3	4	28	24	4	2	20	16				
1	9	41	40	6	9	20	19	4	0	26	26	3	5	15	16	4	3	21	15				
1	10	14	14	7	0	13	11	4	3	23	23	3	6	26	21	4	4	11	10				
1	11	27	29	7	2	17	16	4	5	21	23	3	9	38	35	4	6	16	16				
1	12	21	20	7	3	25	24	4	8	46	44	3	10	9	5	5	0	31	27				
2	0	63	57	7	5	18	14	4	9	18	17	4	0	9	12	5	2	10	8				
2	1	14	16	7	6	28	16	5	0	11	15	4	1	31	30	5	3	8	8				
2	2	53	49	7	9	9	10	5	1	23	25	4	2	20	21	6	0	30	27				
2	4	27	28	8	0	20	29	5	3	16	16	4	4	11	9	6	1	20	17				
2	5	9	8	8	2	20	17	5	4	12	11	4	5	25	25	6	3	15	14				
2	6	9	7	8	3	18	9	5	6	21	20	4	6	32	31	6	4	11	8				
2	7	18	21	8	4	24	24	5	7	15	17	4	7	17	10	7	1	12	11				
2	8	19	19	8	7	11	12	5	9	14	16	4	8	20	19	7	2	31	27				
2	9	19	21	8	8	9	5	5	10	32	30	5	0	28	24								
2	10	27	24	9	1	18	17	6	0	7	8	5	1	22	23	H= 16							
2	12	8	5	9	2	15	14	6	2	16	18	5	5	8	10								
2	13	16	17	9	5	23	23	6	3	18	20	5	6	16	16	0	8	43	37				
2	14	17	14	10	0	15	15	6	4	30	30	5	8	23	19	0	4	21	17				
3	0	19	21	10	1	13	11	6	5	23	22	6	0	15	15	1	1	45	39				
3	1	19	31	10	2	12	16	6	6	14	14	6	1	24	23	1	2	11	8				
3	3	41	45					6	9	24	22	6	2	34	32	1	3	11	8				
3	4	7	1	H= 13				7	0	24	22	6	3	8	2	1	4	12	7				
3	6	24	21					7	1	12	8	6	5	21	22	1	5	8	7				
3	7	14	13	0	8	19	14	7	2	16	15	6	7	24	23	2	0	14	10				
3	8	9	9	0	2	28	19	7	3	19	10	7	0	31	29	2	2	37	35				
3	9	32	31	0	4	18	18	7	4	36	34	7	2	21	21	2	3	11	10				
3	10	11	6	0	6	9	2	8	2	23	22	7	4	25	25	2	6	10	10				
4	0	15	15	0	8	54	51	8	3	21	20	7	5	8	0	3	0	16	12				
4	1	8	5	0	10	8	8	8	5	12	14	8	0	11	10	3	1	14	27				
4	2	29	30	0	12	42	39	9	0	13	10	8	1	21	21	3	4	21	16				
4	4	24	26	1	0	20	15									3	5	8	8				
4	6	8	10	1	1	46	47	H= 14				H= 15				4	0	26	21				
4	7	15	13	1	2	22	21									5	1	23	18				
4	8	14	15	1	3	20	18	0	0	13	15	0	8	58	53								
4	9	13	12	1	4	19	19	0	2	42	39	0	2	16	14	H= 17							
4	10	39	37	1	5	12	13	0	6	28	26	0	8	12	14								
4	11	8	9	1	7	33	31	0	8	18	16	1	0	18	6	0	2	16	17				
4	13	18	9	1	9	18	19	0	10	38	35	1	1	32	29	0	4	21	17				
5	0	18	17	1	10	22	21	1	0	8	11	1	3	27	23	2	0	24	20				
5	2	26	26	1	11	31	28	1	1	31	32	1	4	9	4	2	3	9	5				
5	3	18	19	2	0	47	45	1	2	14	14	1	5	10	7								

Table B. Observed (FO) and Calculated (FC) Structure Factors for $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_4$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
		M=	W																												
0	2	271	281	5	4	97	97	11	5	133	134	17	5	50	64	23	4	31	24	29	10	47	43	6	14	26	20	11	4	83	89
0	4	98	74	5	10	19	17	11	6	64	64	17	4	61	59	25	2	24	21	2	11	19	14	7	6	86	74	11	5	60	65
0	6	264	236	5	13	21	16	11	8	75	81	17	6	21	19	25	1	35	31	2	12	18	14	7	1	71	53	11	6	50	47
0	8	92	82	6	2	48	51	11	9	64	88	17	7	31	29	25	5	57	55	2	13	47	44	7	2	107	99	11	7	95	99
0	10	30	24	6	4	95	101	11	10	33	29	17	8	47	47	25	8	23	21	3	0	314	333	7	3	84	85	11	8	46	53
0	12	21	31	6	5	28	31	11	12	36	34	17	11	31	33	26	1	62	60	3	1	111	112	7	4	46	50	11	9	52	54
0	14	95	92	6	6	25	23	12	0	203	195	17	12	34	32	26	2	24	20	3	2	50	52	7	5	31	27	11	10	29	26
1	2	64	70	6	7	26	28	12	1	164	101	17	13	23	16	26	3	52	46	3	3	54	61	7	6	45	37	11	11	33	34
1	3	61	63	6	8	47	45	12	2	21	25	18	0	110	107	26	4	60	54	3	4	86	90	7	7	30	37	11	12	34	34
1	4	24	35	6	9	40	41	12	3	36	42	18	1	68	64	26	5	21	13	3	5	44	99	7	8	40	40	11	13	34	31
1	5	47	59	6	10	28	36	12	4	73	87	18	2	40	37	27	6	24	24	3	6	61	62	7	9	25	25	11	14	34	32
1	7	73	73	6	11	41	39	12	5	166	108	18	3	46	55	27	7	31	32	3	7	22	14	7	10	35	38	12	0	29	60
1	8	56	62	7	1	63	52	12	6	54	59	18	4	17	16	27	8	28	27	3	8	68	68	7	11	38	34	12	1	145	143
1	10	152	142	7	2	46	37	12	7	114	119	18	5	30	27	28	9	84	81	3	9	73	76	7	12	34	37	12	2	61	62
1	12	46	41	7	3	70	59	12	8	42	43	18	6	47	45	28	10	70	62	3	10	40	43	7	13	31	31	12	3	69	61
1	13	47	41	7	4	28	14	12	9	103	100	18	7	19	18	28	11	21	21	3	11	19	21	8	0	293	265	12	4	85	86
2	2	187	187	7	5	80	86	12	10	39	41	18	8	39	38	28	0	22	22	3	12	24	29	8	1	109	109	12	5	52	47
2	3	122	118	7	6	30	46	13	12	38	29	18	11	39	38	30	1	60	58	3	14	46	45	8	2	85	74	12	6	82	82
2	4	183	174	7	7	52	46	13	3	84	74	19	1	22	15	30	2	21	25	3	15	21	23	8	3	50	54	12	7	34	46
2	5	53	42	7	8	85	90	13	4	32	30	19	2	64	63	30	3	21	25	4	0	29	23	8	4	84	87	12	8	75	79
2	6	60	67	7	12	21	15	13	5	71	74	19	3	28	27	30	4	14	14	4	1	45	84	8	5	86	73	12	9	52	52
2	7	20	10	8	0	221	210	13	6	55	61	19	4	24	22	30	5	14	14	4	2	80	77	8	6	27	27	12	10	38	38
2	8	67	69	8	1	39	54	13	7	19	10	19	5	24	19	30	6	14	14	4	3	57	49	8	8	80	80	12	12	24	22
2	9	17	24	8	2	22	28	13	8	97	103	19	6	29	26	30	7	85	80	4	4	65	68	8	9	52	53	12	13	44	45
2	10	51	50	8	3	110	99	13	9	40	43	19	7	28	27	30	8	144	145	4	5	91	92	8	10	33	36	13	0	36	44
2	13	72	70	8	4	17	24	14	0	173	172	20	0	84	92	30	9	144	145	4	6	26	31	8	13	28	31	13	1	153	146
2	15	47	44	8	5	26	15	14	1	40	40	20	1	44	44	30	10	14	14	4	7	76	79	9	0	174	177	13	5	61	68
3	1	82	88	8	6	65	70	14	2	136	139	20	2	33	37	30	11	34	32	4	8	79	80	9	1	116	119	13	4	78	74
3	2	13	3	8	8	62	63	14	3	129	137	20	3	20	21	30	12	34	32	4	9	104	99	9	2	30	29	13	5	98	101
3	4	12	5	8	10	44	45	14	4	111	109	20	4	25	29	30	13	34	32	4	10	58	65	9	3	63	72	13	6	112	113
3	5	104	106	8	12	36	40	14	5	21	24	21	5	42	39	30	14	41	44	4	12	34	35	9	4	54	60	13	7	35	35
3	6	32	45	9	14	33	27	14	6	62	66	21	6	33	32	30	15	34	32	4	13	23	21	9	5	77	80	13	8	87	89
3	8	142	144	9	16	33	25	14	7	24	19	21	7	43	41	30	16	34	32	4	14	31	36	5	1	105	99	13	9	70	71
3	9	28	27	9	18	33	35	14	8	62	66	21	8	33	30	30	17	34	32	4	15	31	36	5	2	33	37	13	10	40	42
3	10	64	66	9	20	33	35	14	9	24	19	21	9	40	44	30	18	34	32	4	16	31	36	5	3	50	52	13	11	36	36
3	11	20	23	9	22	33	35	14	10	62	66	21	10	40	44	30	19	34	32	4	17	31	36	5	4	35	42	14	0	107	107
3	12	35	26	9	24	33	35	14	11	28	25	21	11	28	25	30	20	34	32	4	18	31	36	5	5	52	56	14	1	71	69
4	0	174	173	9	26	33	35	14	12	32	35	21	12	28	25	30	21	34	32	4	19	31	36	5	6	29	35	14	2	29	35
4	1	94	91	9	28	33	35	14	13	16	12	21	13	33	33	30	22	34	32	4	20	31	36	5	7	35	30	14	3	88	79
4	2	33	29	9	30	33	35	14	14	16	12	21	14	33	33	30	23	34	32	4	21	31	36	5	8	44	53	14	4	45	48
4	3	80	87	9	32	33	35	14	15	16	12	21	15	33	33	30	24	34	32	4	22	31	36	5	9	60	64	14	5	71	69
4	4	33	29	9	34	33	35	14	16	16	12	21	16	33	33	30	25	34	32	4	23	31	36	5	10	24	23	14	6	39	44
4	5	80	87	9	36	33	35	14	17	16	12	21	17	33	33	30	26	34	32	4	24	31	36	5	11	34	32	14	7	16	13
4	6	33	29	9	38	33	35	14	18	16	12	21	18	33	33	30	27	34	32	4	25	31	36	5	12	24	25	14	8	65	65
4	7	33	29	9	40	33	35	14	19	16	12	21	19	33	33	30	28	34	32	4	26	31	36	5	13	34	32	14	9	35	33
4	8	33	29	9	42	33	35	14	20	16	12	21	20	33	33	30	29	34	32	4	27	31	36	5	14	34	32	14	10	34	38
4	9	33	29	9	44	33	35	14	21	16	12	21	21	33	33	30	30	34	32	4	28	31	36	5	15	34	32	14	11	29	29
4	10	21	30	9	46	33	35	14	22	16	12	21	22	33	33	30	31	34	32	4	29	31	36	5	16	34	32	14	12	29	29
4	11	30	30	9	48	33	35	14	23	16	12	21	23	33	33	30	32	34	32	4	30	31	36	5	17	34	32	14	13	29	29
4	12	30	30	9	50	33	35	14	24	16	12	21	24	33	33	30	33	34	32	4	31	31	36	5	18	34	32	14	14	29	29
4	13	30	30	9	52	33	35	14	25	16	12	21	25	33	33	30	34	34	32	4	32	31	36	5	19	34	32	14	15	29	29
4	14	30	30	9	54	33	35	14	26	16	12	21	26	33	33	30	35	34	32	4	33	31	36	5	20	34	32	14	16	29	29
4	15	24	20	9	56	33	35	14	27	16	12	21	27	33	33	30	36	34	32	4	34	31	36	5	21	34	32	14	17	29	29
5	1	97	91	9	58	33	35	14	28	16	12	21	28	33	33	30	37	34													

Table B. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
15	10	54	50	23	4	44	40	1	4	115	121	5	4	90	95	9	6	51	44	13	13	29	29	19	6	52	52	26	4	40	41
16	1	52	51	23	5	20	26	1	5	144	140	5	5	72	74	9	8	79	73	14	0	103	109	19	7	19	24	26	5	23	23
16	2	91	91	23	7	40	50	1	6	121	115	5	6	41	34	9	9	51	54	14	1	45	52	19	8	40	43	26	6	23	14
16	3	43	39	23	9	21	16	1	7	141	152	5	7	102	98	9	10	32	31	14	2	44	46	19	9	31	28	26	7	23	24
16	4	50	60	24	1	25	23	1	8	94	95	5	8	47	44	9	11	14	17	14	3	61	63	19	12	26	22	27	2	24	25
16	5	33	30	24	2	16	19	1	9	110	116	5	9	88	85	9	12	25	24	14	4	65	63	20	0	29	31	27	3	33	34
16	7	37	32	24	3	31	34	1	10	47	40	5	10	32	36	9	11	58	54	14	5	129	131	20	1	31	32	27	5	33	34
16	9	39	16	24	4	45	43	1	11	56	61	5	11	45	44	9	14	22	24	14	6	52	53	20	2	18	20	27	7	23	18
16	11	22	17	24	5	47	49	1	12	32	34	6	0	21	25	10	1	104	109	14	7	44	42	20	4	34	35	26	0	37	35
16	13	40	35	24	6	37	36	1	13	42	46	6	1	70	64	10	1	142	145	14	8	56	50	20	5	23	21	24	2	20	19
17	0	149	148	24	8	22	18	1	14	22	23	6	2	34	38	10	2	52	55	14	9	31	34	20	6	35	30	28	3	36	17
17	1	16	20	24	9	34	34	2	0	184	194	6	3	40	33	10	3	57	66	14	10	24	22	20	9	19	19	28	5	37	32
17	2	31	24	25	0	40	40	2	1	62	61	6	4	67	57	10	4	36	32	14	11	23	19	21	0	30	27	29	3	25	17
17	3	62	50	25	2	27	23	2	2	38	39	6	5	42	36	10	5	66	62	14	12	30	25	21	1	45	47	29	4	22	20
17	4	43	37	25	3	67	60	2	3	85	84	6	6	69	60	10	6	29	21	15	0	27	20	21	2	53	53	30	1	23	23
17	5	45	45	25	4	32	30	2	4	215	208	6	7	20	19	10	6	64	67	15	1	75	76	21	3	18	16				
17	6	37	40	25	5	28	27	2	5	106	92	6	8	40	40	10	7	16	12	15	2	47	49	21	4	26	29				
17	7	35	31	25	6	47	43	2	6	118	123	6	9	40	40	10	11	26	20	15	3	120	120	21	5	41	39				
17	8	25	25	25	8	26	26	2	7	36	48	6	10	31	29	10	12	27	20	15	4	61	60	21	6	20	22	0	1	140	142
17	9	56	54	26	4	35	33	2	8	44	46	6	11	26	28	10	13	46	45	15	5	32	30	21	7	48	50	0	2	196	183
17	11	20	21	26	5	22	24	2	9	89	84	6	12	23	25	11	0	103	101	19	6	29	28	21	8	30	27	0	3	60	49
17	11	42	40	26	7	21	15	2	10	45	45	6	13	23	25	11	1	31	30	19	6	50	44	21	9	28	32	0	4	136	144
18	2	60	75	26	8	33	35	2	11	19	16	7	0	183	179	11	2	130	145	15	9	47	49	22	0	59	60	0	5	63	73
18	3	52	51	27	0	33	30	2	13	43	39	7	1	76	74	11	3	24	25	15	10	24	20	22	1	41	44	0	6	160	154
18	7	36	34	27	1	50	52	2	14	31	36	7	2	53	47	11	4	64	60	15	11	21	14	22	2	25	20	0	7	170	179
18	7	40	49	27	2	54	51	3	0	17	9	7	3	116	116	11	5	46	45	16	0	84	77	22	7	21	20	0	8	32	25
18	8	35	37	27	4	41	44	3	1	19	18	7	4	65	65	11	6	44	40	16	1	68	60	22	8	24	23	0	9	65	77
18	9	39	35	27	5	25	26	3	2	50	45	7	5	81	80	11	7	21	23	16	2	44	44	23	0	59	60	0	10	31	31
18	12	30	34	28	5	26	28	3	3	58	53	7	6	30	36	11	8	53	49	16	4	100	96	23	1	24	22	0	11	54	59
19	0	26	32	29	0	54	51	3	4	126	141	7	7	39	39	11	9	20	24	16	5	43	36	23	2	20	19	0	11	69	71
19	1	62	66	29	1	40	36	3	5	37	35	7	8	52	50	11	10	29	30	16	6	51	50	23	3	21	23	0	15	21	20
19	4	36	37	29	2	24	30	3	6	136	132	7	9	79	84	11	13	31	34	16	8	23	23	23	4	37	37	1	0	50	47
19	10	28	25	29	3	30	30	3	7	56	62	7	10	44	49	11	14	41	42	16	9	29	28	23	5	41	42	1	1	33	31
20	0	21	21					3	8	135	130	7	11	30	31	12	0	166	173	16	10	25	20	23	6	37	40	1	2	39	36
20	1	50	50					3	9	30	33	7	13	25	25	12	1	85	74	16	13	25	25	23	7	24	25	1	3	78	85
20	2	27	22					3	10	81	82	7	14	31	31	12	2	82	71	17	0	66	69	23	8	32	30	1	4	199	206
20	3	37	37					3	12	37	36	8	0	105	113	12	3	43	46	17	2	106	101	23	9	30	35	1	5	168	160
20	4	34	31					3	13	36	28	8	1	90	82	12	4	115	115	17	3	28	30	23	10	21	20	1	6	43	38
20	5	35	39					4	0	47	42	8	2	108	98	12	5	68	71	17	4	49	51	24	1	44	43	1	8	65	62
20	7	20	21					4	1	121	114	8	3	27	37	12	6	50	48	17	7	28	20	24	3	40	40	1	9	58	56
20	8	50	50					4	2	56	44	8	4	27	24	12	7	31	34	17	8	47	43	24	4	22	24	1	10	56	56
20	11	24	25					4	3	49	50	8	5	35	31	12	9	60	70	17	12	25	22	24	5	20	30	1	11	26	28
21	0	35	38					4	4	72	71	8	6	32	29	12	10	23	21	18	0	50	55	24	6	26	22	2	0	15	34
21	2	21	26					4	5	135	121	8	7	39	39	12	11	14	16	14	1	46	49	24	7	19	18	2	1	39	38
21	6	24	27					4	6	39	34	8	8	36	35	12	12	40	37	14	2	30	21	24	8	21	23	2	2	86	84
21	4	19	14					4	7	33	38	8	9	42	35	12	13	21	14	14	3	42	38	25	0	35	33	2	3	142	154
22	1	54	54					4	8	69	78	8	11	19	20	12	14	23	20	14	5	54	61	25	2	29	20	2	4	232	215
22	1	23	26					4	9	55	53	8	12	35	37	13	0	33	37	14	6	27	20	25	3	20	18	2	5	118	114
22	2	46	46					4	10	22	18	8	13	25	25	13	1	130	131	14	9	25	23	25	4	57	53	2	6	118	114
22	4	24	24					4	11	31	24	8	14	26	29	13	2	90	96	14	11	22	20	25	5	34	31	2	7	22	29
22	5	50	54					4	12	42	35	9	0	70	64	13	3	77	80	14	12	24	18	25	6	31	26	2	8	119	118
22	9	31	24					4	13	20	27	9	1	220	218	13	4	94	93	14	0	47	53	25	8	37	30	2	9	64	58
22	7	20	33					5	1	31	23	9	2	46	42	13	5	99	92	14	1	62	60	26	1	40	43	2	10	39	47
22	7	30	38					5	1	86	75	9	3	36	30	13	7	29	27	14	2	46	47	26	1	29	25	2	11	25	29
23	1	40	45					5	2	77	72	9	4	73	61	13	8	31	39	14	3	55	55	26	2	36	36	2	12	55	55
23	1	29	27					5	3	77	80	9	5	24	19	13	9	75	71	13	5	21	25	26	3	24	26	2	14	37	41

Table B. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
3	1	48	37	7	0	28	38	11	6	44	47	16	3	83	86	21	2	36	42	2	2	112	100	6	7	67	72	13	5	40	43
3	1	94	94	7	1	52	53	11	7	60	67	16	4	110	110	21	3	22	23	2	3	113	107	6	8	37	41	13	6	24	22
3	2	17	4	7	2	76	74	11	8	59	53	16	5	53	51	21	4	22	20	2	4	146	148	6	9	49	49	13	7	29	31
3	3	59	69	7	4	30	32	11	9	63	60	16	7	21	19	21	3	21	22	2	5	142	148	6	10	36	35	13	8	34	31
3	4	97	92	7	5	73	69	11	11	22	24	16	9	35	37	21	1	39	40	2	6	53	43	6	11	30	31	13	10	35	35
3	5	138	136	7	6	33	33	11	12	38	31	16	10	28	27	21	3	30	32	2	8	64	52	6	12	31	37	13	11	35	31
3	6	63	61	7	7	53	59	11	14	22	17	16	11	26	26	21	4	57	55	2	9	46	45	6	14	34	26	13	12	40	38
3	7	75	77	7	8	79	73	12	1	44	54	17	0	51	56	21	6	40	39	2	10	37	39	7	5	85	84	14	5	77	78
3	10	17	16	7	9	27	25	12	1	137	143	17	2	38	36	21	8	26	23	2	11	20	21	7	6	15	10	14	6	51	48
3	11	18	10	7	12	42	44	12	2	75	81	17	3	45	52	21	1	26	27	2	12	24	21	7	7	50	55	14	7	35	36
3	12	38	40	7	13	22	24	12	3	74	75	17	4	41	45	25	0	37	39	2	14	24	20	7	9	24	25	14	8	48	42
3	14	23	19	7	14	23	18	12	4	84	87	17	5	73	75	25	1	53	52	3	0	32	35	7	10	44	43	14	9	64	65
3	15	21	21	8	0	34	55	12	5	55	55	17	6	30	25	25	2	30	35	3	1	56	45	7	11	29	25	14	10	58	56
4	1	46	51	8	1	104	99	12	6	28	32	17	7	43	39	25	3	20	25	3	2	72	70	7	12	35	32	14	12	48	46
4	1	144	137	8	3	55	51	12	7	41	33	17	9	43	47	25	4	24	20	3	3	120	119	7	13	25	23	15	5	59	60
4	2	18	6	8	4	73	71	12	8	37	32	18	0	82	79	26	1	51	51	3	4	109	103	7	14	29	28	15	6	35	40
4	3	59	68	8	5	31	38	12	9	50	48	18	1	45	43	26	4	19	15	3	5	146	102	8	5	67	67	15	7	28	29
4	4	147	191	8	6	20	23	12	11	24	21	18	2	56	58	26	3	39	35	3	6	41	48	8	6	114	113	15	9	29	27
4	4	142	191	8	7	31	30	12	13	41	38	18	3	80	85	27	0	29	10	3	7	37	35	8	7	41	41	15	10	32	30
4	5	20	18	8	8	57	56	13	0	49	55	18	4	32	39	27	1	26	27	3	8	35	42	8	8	83	79	15	11	34	31
4	6	58	52	8	10	70	70	13	1	93	102	18	5	20	21	27	2	22	22	3	10	45	41	8	9	46	52	15	12	31	25
4	7	90	87	8	11	31	38	13	2	20	22	18	6	29	25	27	1	27	24	3	11	29	26	8	10	35	39	16	6	36	34
4	8	26	31	8	13	59	56	13	3	73	70	18	7	26	23	27	4	33	31	3	12	26	29	8	12	36	35	16	7	20	25
4	9	55	56	9	0	54	56	13	4	113	119	18	8	20	17	28	2	37	36	3	13	41	44	9	5	45	43	16	8	62	58
4	10	67	65	9	1	67	73	13	5	58	59	18	9	20	13	28	4	31	31	4	0	62	71	9	6	54	52	16	9	43	45
4	11	25	27	9	2	25	24	13	6	75	76	18	12	34	31	29	2	36	32	4	1	156	145	9	7	36	27	16	10	29	29
4	12	25	25	9	3	74	66	13	8	67	64	19	0	28	31	4	2	88	85	4	2	88	85	9	8	33	36	16	11	48	48
4	13	24	18	9	4	59	53	13	10	51	50	19	1	28	25	4	3	162	167	4	3	162	167	9	9	43	38	17	5	38	33
5	0	169	161	9	5	50	56	13	11	38	35	19	3	18	10	4	4	126	128	4	4	126	128	9	10	31	29	17	7	22	19
5	1	73	63	9	6	77	79	13	13	21	21	19	4	58	66	4	5	90	83	4	5	90	83	9	12	23	29	17	8	20	15
5	2	93	47	9	7	53	55	14	0	29	40	19	5	23	22	4	6	48	47	4	6	48	47	9	13	43	43	17	10	37	33
5	3	46	34	9	8	54	54	14	1	54	60	19	6	48	49	4	7	16	20	4	7	16	20	9	14	23	28	17	11	31	28
5	4	74	86	9	9	53	52	14	2	72	75	19	7	18	20	4	8	58	51	4	8	58	51	10	5	93	96	18	5	61	63
5	5	93	82	9	10	37	38	14	3	119	124	19	8	40	37	4	9	23	22	4	9	23	22	10	6	69	68	18	7	53	51
5	6	21	23	9	11	24	22	14	4	71	75	20	1	63	65	4	10	23	25	4	10	23	25	10	7	104	105	18	8	20	22
5	7	30	35	9	13	28	29	14	5	65	63	20	2	24	28	4	11	50	51	4	11	50	51	10	8	77	73	18	9	35	39
5	8	52	45	9	14	26	23	14	6	48	47	20	3	28	30	4	13	34	37	4	13	34	37	10	9	55	60	18	10	41	37
5	9	40	36	10	0	172	180	14	8	65	60	20	4	34	37	4	14	127		4	14	127		10	10	37	40	19	6	33	31
5	11	42	44	10	1	98	98	14	10	34	37	20	7	27	25	4	15	84	80	4	15	84	80	10	11	31	31	19	11	21	15
5	12	29	29	10	2	90	84	14	12	20	19	20	8	32	35	4	16	26	27	4	16	26	27	11	5	81	81	20	5	23	25
5	13	34	32	10	3	14	12	15	0	22	22	21	0	43	46	4	17	19	131	4	17	19	131	11	6	50	50	20	6	56	55
5	14	24	23	10	4	53	52	15	1	35	34	21	1	35	39	4	18	59	51	4	18	59	51	11	7	42	41	20	8	48	45
6	1	74	76	10	6	42	46	15	2	26	28	21	2	21	21	4	19	25	22	4	19	25	22	11	8	29	28	20	9	42	37
6	1	41	41	10	7	31	36	15	3	32	34	21	3	40	44	4	20	21	25	4	20	21	25	11	9	39	35	20	10	21	24
6	2	23	37	10	8	46	42	15	4	84	84	21	4	25	24	4	21	47	51	4	21	47	51	11	10	27	22	21	5	25	23
6	3	101	105	10	9	53	46	15	5	82	82	21	5	38	35	4	22	31	37	4	22	31	37	11	11	25	28	21	7	23	17
6	4	38	43	10	10	26	22	15	6	44	46	22	0	47	45	4	23	46	56	4	23	46	56	11	12	34	36	22	5	35	32
6	5	58	56	10	12	57	51	15	8	38	38	22	2	27	22	4	24	20	44	4	24	20	44	11	13	42	43	22	7	32	29
6	6	34	44	10	13	29	28	15	9	43	39	22	4	22	19	4	25	24	26	4	25	24	26	12	5	119	124	22	8	44	44
6	7	49	46	10	14	51	44	15	10	27	26	22	5	43	44	4	26	27	24	4	26	27	24	12	6	79	86	22	9	20	23
6	8	72	61	11	0	168	166	15	11	40	41	22	7	42	36	4	27	49	43	4	27	49	43	12	7	43	44	22	5	24	26
6	9	17	17	11	1	22	28	15	12	25	23	22	8	20	19	4	28	44	41	4	28	44	41	12	8	70	74	23	6	24	22
6	11	24	28	11	2	77	81	15	13	25	20	22	9	23	31	4	29	43	27	4	29	43	27	12	9	71	68	23	7	22	23
6	12	18	20	11	3	17	75	16	1	49	38	22	10	22	19	4	30	38	38	4	30	38	38	12	10	21	26	24	6	22	14
6	13	28	23	11	4	28	31	16	2	53	50	23	1	53	54	4	31	24	23	4	31	24	23	12	11	43	41	24	7	22	19

Table B. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
25	7	22	22	4	0	58	62	8	12	20	27	13	12	27	25	20	0	21	24	1	0	115	108	5	4	40	41	9	12	30	28
25	8	23	16	4	1	27	34	9	0	21	11	14	1	112	117	20	4	14	16	1	1	59	67	5	5	47	47	10	0	30	29
26	5	32	30	4	2	09	82	9	1	40	41	14	2	53	53	21	0	63	65	1	2	36	41	5	6	29	33	10	1	79	80
27	6	25	19	4	3	77	70	9	2	16	10	14	3	24	21	21	1	41	37	1	3	70	65	5	7	43	42	10	2	49	54
				4	4	05	66	9	3	117	117	14	4	45	41	21	2	53	49	1	4	94	107	5	9	41	42	10	3	54	51
				4	5	55	54	9	4	28	30	14	5	22	26	21	4	45	45	1	5	69	67	5	10	23	24	10	4	126	124
				4	6	31	37	9	5	134	130	14	6	73	29	21	5	33	30	1	6	90	89	5	11	61	61	10	5	44	50
				4	7	18	17	9	6	107	104	14	10	30	35	21	0	41	43	1	7	79	71	5	12	34	40	10	7	38	39
				4	8	16	10	9	7	35	34	14	12	40	42	21	7	33	35	1	8	52	53	5	13	36	37	10	8	27	35
				4	10	35	35	9	8	72	70	15	1	44	44	21	8	46	36	1	9	41	43	5	14	33	29	10	10	35	33
				4	11	27	24	9	9	46	48	15	2	27	24	21	9	26	26	1	10	34	32	6	0	31	42	10	11	20	20
				4	12	56	53	9	10	18	16	15	3	33	29	21	11	25	25	1	11	37	34	6	1	23	30	10	13	21	25
				4	14	35	34	9	11	33	29	15	4	53	54	22	1	52	45	1	14	25	23	6	2	50	54	11	0	31	39
				5	0	88	79	10	0	30	23	15	5	19	22	22	2	27	24	2	0	75	72	6	3	113	104	11	1	61	59
				5	1	19	18	10	1	34	39	15	7	34	35	22	3	19	17	2	1	63	63	6	4	46	49	11	2	104	96
				5	2	100	105	10	2	24	22	15	8	21	27	22	4	19	19	2	2	22	23	6	5	107	110	11	3	10	29
				5	3	111	123	10	3	55	60	15	9	39	42	22	5	32	30	2	3	72	74	6	6	45	44	11	4	76	82
				5	4	99	95	10	4	121	127	15	10	59	58	22	9	22	23	2	4	17	24	6	7	28	27	11	5	80	84
				5	5	06	87	10	5	31	33	15	11	30	28	22	0	31	33	2	5	48	48	6	9	47	53	11	6	26	27
				5	6	27	31	10	6	69	65	16	0	130	124	23	1	27	30	2	6	16	9	6	10	46	52	11	7	25	24
				5	8	53	60	10	7	29	29	16	1	40	42	23	2	43	42	2	7	66	69	6	11	21	16	11	8	21	25
				5	9	63	63	10	8	21	19	16	2	57	63	23	3	23	26	2	8	30	39	7	0	28	27	11	9	26	24
				5	10	26	23	10	9	24	23	16	3	58	59	23	4	32	32	2	9	31	34	7	1	59	57	11	12	24	25
				5	11	53	54	10	10	24	26	16	5	22	23	23	5	48	46	2	10	25	28	7	2	67	65	11	13	23	19
				5	12	24	25	10	12	26	25	16	7	33	36	23	7	36	35	2	11	19	18	7	3	72	67	12	0	85	80
				5	13	22	18	11	1	42	43	16	11	43	36	24	0	50	54	2	12	29	30	7	4	53	55	12	2	29	28
				6	0	18	13	11	2	23	22	16	12	29	25	24	4	36	33	2	13	23	22	7	5	69	70	12	3	64	79
				6	1	28	27	11	3	46	49	17	1	20	21	25	1	32	29	2	14	25	22	7	6	21	22	12	4	26	21
				6	2	48	50	11	4	93	90	17	2	51	49	25	1	40	41	3	1	54	54	7	7	40	50	12	5	67	73
				6	3	76	74	11	5	101	99	17	3	58	60	25	4	27	27	3	2	103	101	7	8	27	24	12	6	39	38
				6	4	56	61	11	6	59	61	17	4	25	25	26	1	38	24	3	4	55	56	7	9	26	24	12	8	23	25
				6	5	59	59	11	7	91	88	17	5	49	50	26	2	20	22	3	5	78	82	7	10	38	37	12	9	35	37
				6	6	24	18	11	8	34	34	17	6	22	19	26	3	29	29	3	6	58	59	7	11	26	29	12	10	24	25
				6	7	20	26	11	9	65	70	17	7	32	37	26	5	21	25	3	7	65	60	7	12	36	34	12	11	88	88
				6	11	24	26	11	11	22	19	17	9	54	54	26	6	35	28	3	8	69	68	7	13	27	24	13	1	103	102
				6	12	24	18	11	13	29	26	17	10	27	24	27	2	29	28	3	9	27	37	8	0	50	49	13	2	49	53
				6	13	42	41	12	0	82	85	17	11	26	30	27	4	26	23	3	10	39	42	8	2	06	88	13	3	74	73
				7	0	38	41	12	1	35	33	18	0	45	45	27	5	24	18	3	12	56	59	8	3	106	105	13	4	36	34
				7	1	59	53	12	2	91	95	18	1	77	79	28	0	28	23	3	13	35	35	8	4	93	82	13	7	19	21
				7	2	00	67	12	3	87	86	18	2	61	67	28	1	37	36	4	0	17	25	8	5	78	75	13	11	32	34
				7	3	70	78	12	4	26	33	18	3	37	38	28	2	37	38	4	1	56	47	8	6	80	81	13	12	30	28
				7	4	135	137	12	5	77	75	18	4	48	42	28	3	28	25	4	2	75	88	8	7	20	29	14	0	26	21
				7	5	30	35	12	10	22	17	18	7	27	26	28	4	28	25	4	3	91	99	8	8	25	25	14	1	24	20
				7	6	63	62	12	11	44	44	19	1	64	62	28	5	26	25	4	4	82	72	8	9	31	36	14	2	19	13
				7	7	77	73	12	13	28	28	19	3	37	37	28	6	26	24	4	5	28	32	8	10	33	30	14	3	33	30
				7	8	61	70	13	0	23	22	19	4	51	48	28	7	22	21	4	6	39	50	8	11	35	32	14	4	55	56
				7	10	64	54	13	1	31	28	19	5	47	52	28	8	20	20	4	7	37	40	8	12	26	27	14	5	16	9
				7	12	28	27	13	2	31	27	19	6	47	46	28	9	19	19	4	8	41	51	9	1	38	39	14	6	24	32
				8	0	19	14	13	3	52	59	19	7	29	28	28	10	18	18	4	9	22	25	9	2	67	60	14	7	30	28
				8	1	28	36	13	4	66	67	19	8	45	46	28	11	17	17	4	10	45	44	9	3	70	71	14	9	35	39
				8	2	36	29	13	5	25	24	19	9	30	28	28	12	14	14	4	11	55	55	9	4	94	92	14	10	38	39
				8	3	36	37	13	6	38	42	19	10	35	34	28	13	22	24	4	12	22	24	9	5	58	65	15	1	90	90
				8	4	05	63	13	7	61	65	20	0	43	32	28	14	23	24	5	0	112	109	9	6	63	64	15	1	77	74
				8	5	84	86	13	9	27	32	20	1	38	47	28	15	29	25	5	1	63	63	9	8	20	27	15	2	59	61
				8	7	18	18	13	10	41	45	20	2	32	41	28	16	32	31	5	2	67	74	4	10	29	28	15	3	52	54
				8	8	35	38	13	11	36	36	20	3	32	24	28	17	22	21	5	3	25	29	4	11	25	23	15	4	18	9

Table B. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
15	0	23	41	23	0	21	24	3	0	56	61	8	2	37	30	13	0	19	18	22	2	26	25	4	2	142	102	8	12	20	18
15	8	24	23	23	1	24	23	3	7	22	24	8	3	89	88	13	10	23	24	22	1	20	19	4	3	36	36	9	0	23	19
15	11	24	22	23	2	27	24	3	4	62	64	8	4	16	21	14	0	20	24	22	4	34	32	4	4	34	35	9	1	24	27
15	12	37	38	23	5	21	23	3	10	38	42	8	5	74	75	14	1	87	84	22	5	24	24	4	5	27	27	9	2	58	62
16	0	33	35	23	6	20	16	3	12	26	30	8	6	27	32	14	2	36	34	22	6	32	27	4	6	34	38	9	4	43	43
16	1	33	35	23	8	25	22	4	0	85	93	8	7	49	47	14	3	44	42	23	1	32	33	4	8	45	43	9	5	21	20
16	2	27	26	24	2	26	23	4	1	64	63	8	8	25	26	14	4	20	14	23	1	21	17	4	10	34	32	9	6	40	38
16	3	66	67	24	3	27	27	4	2	82	82	8	10	44	47	14	6	35	34	23	1	49	46	4	12	22	25	9	7	44	52
16	5	27	25	24	4	52	47	4	3	26	33	8	11	27	25	14	7	26	31	23	5	44	44	5	0	79	80	9	8	42	44
16	6	18	18	24	5	22	23	4	4	47	43	8	12	42	39	14	11	32	14	24	0	39	38	5	1	40	21	9	11	24	24
16	8	24	10	25	0	21	19	4	5	61	64	9	0	96	88	15	1	42	43	24	2	28	32	5	2	100	97	9	12	39	40
16	9	37	35	25	1	38	37	4	6	19	23	9	1	36	33	15	2	33	35	25	1	25	26	5	3	28	26	10	0	79	78
16	11	35	34	25	5	24	20	4	7	42	44	9	3	102	104	15	3	24	23	25	2	21	20	5	4	29	33	10	1	34	39
17	0	76	72	25	6	21	27	4	8	38	37	9	4	53	57	15	4	22	20	25	4	26	28	5	5	49	48	10	2	57	58
17	1	59	60	26	1	28	25	4	9	41	47	9	5	64	64	15	6	37	37	27	0	30	24	5	6	34	31	10	3	70	73
17	2	67	65	27	0	39	37	4	10	53	53	9	7	20	14	15	8	21	16	5	7	28	28	5	7	28	28	10	4	31	36
17	4	32	32					4	11	26	25	9	9	39	39	16	0	76	76					5	8	29	30	10	5	24	20
17	5	33	35					4	12	57	59	9	10	38	41	16	1	32	25					5	9	33	32	10	6	27	24
17	7	25	24					5	0	57	67	9	11	29	35	16	2	41	44					5	10	36	35	10	7	33	33
17	11	20	18					5	1	61	64	10	0	21	21	16	3	18	20					5	11	40	38	10	9	44	41
18	1	38	38					5	2	24	25	10	1	61	62	16	5	46	49					5	12	35	31	10	10	35	30
18	2	60	66					5	3	114	109	10	2	55	58	16	6	29	31					6	0	123	123	10	11	23	26
18	4	56	66					5	4	38	44	10	3	48	49	16	7	31	34					6	1	63	85	11	0	31	28
18	5	41	37					5	5	84	84	10	4	88	86	16	8	28	30					6	2	67	67	11	1	38	39
18	7	41	40					5	7	34	43	10	5	29	29	17	0	32	40					6	3	53	56	11	3	26	30
18	8	32	28					5	8	41	44	10	6	63	67	17	1	29	30					6	4	51	58	11	5	43	48
18	10	37	33					5	9	27	31	10	7	34	36	17	2	24	28					6	5	41	42	11	6	49	46
19	0	28	22					5	10	35	35	10	8	33	35	17	3	30	27					6	7	40	38	11	7	41	44
19	1	41	39					5	11	39	36	10	9	37	39	17	6	37	37					6	9	45	46	11	8	33	39
19	3	45	45					5	13	21	18	10	11	33	35	17	7	23	31					6	10	32	30	11	9	27	22
19	4	37	39					6	0	35	35	11	0	34	32	18	1	37	38					6	11	30	34	11	11	33	29
19	5	41	33					6	1	89	90	11	1	45	50	18	2	22	24					6	12	22	18	12	0	32	31
19	6	30	29					6	2	96	96	11	2	56	57	18	4	55	59					7	0	22	20	12	1	32	33
19	7	33	26					6	3	53	53	11	3	65	59	18	6	54	53					7	1	71	76	12	2	23	23
19	8	21	20					6	4	35	34	11	4	64	62	17	7	25	22					7	2	26	29	12	4	61	67
19	10	23	21					6	5	36	40	11	5	43	51	16	8	31	36					7	3	72	71	12	5	38	37
20	0	27	33					6	6	31	31	11	6	35	36	19	1	23	26					7	4	28	19	12	6	30	26
20	1	22	24					6	7	16	14	11	9	30	34	19	2	23	27					7	5	24	25	12	7	22	26
20	2	21	17					6	8	21	30	11	10	26	28	19	3	57	59					7	6	43	43	12	8	20	22
20	3	43	44					6	9	49	48	11	11	25	20	19	5	47	45					7	7	38	38	12	9	34	37
20	4	29	30					6	10	21	19	12	0	96	97	19	6	20	19					7	8	19	23	12	10	39	37
20	5	44	45					6	11	63	62	12	1	20	21	19	7	25	28					7	9	32	28	12	11	21	22
20	6	49	46					6	12	35	36	12	2	93	92	19	8	26	23					7	10	34	35	13	0	37	40
20	8	22	19					6	13	34	36	12	3	28	31	20	1	32	35					7	11	46	43	13	1	31	33
20	9	32	26					7	0	21	20	12	4	25	27	20	2	25	26					7	12	26	16	13	2	44	47
21	2	22	24					7	1	61	70	12	5	47	52	20	3	49	46					8	0	42	48	13	5	48	47
21	3	34	32					7	2	102	95	12	7	50	47	20	5	62	61					8	1	98	98	13	6	32	38
21	4	30	28					7	3	48	44	12	8	28	36	20	6	40	37					8	2	54	63	13	9	34	34
21	5	32	37					7	4	124	128	12	9	24	24	20	8	34	35					8	3	58	59	13	10	20	21
21	8	25	25					7	6	19	22	12	12	40	39	21	0	26	24					8	4	66	69	14	0	55	58
21	9	30	27					7	9	23	20	13	1	35	35	21	1	21	23					8	5	32	31	14	1	26	24
22	3	32	31					7	10	43	43	13	2	22	18	21	2	42	47					8	6	26	31	14	3	33	36
22	4	30	31					7	11	26	23	13	3	46	46	21	4	61	61					8	8	34	35	14	6	46	52
22	5	47	43					7	12	26	24	13	4	22	31	21	6	32	31					8	9	38	37	14	7	28	24
22	6	32	31					8	1	42	42	13	5	13	20	22	7	28	28					8	10	42	44	14	8	52	50
22	7	39	39					8	1	70	71	13	7	34	32	22	1	31	32					8	11	32	28	14	9	23	23

Table B. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
15	0	26	31	23	5	22	15	5	4	16	3	10	8	29	31	13	5	22	20	5	2	17	13	12	6	25	30	2	7	47	45	2	7	47	45
15	1	23	27	24	0	29	30	5	5	20	25	10	9	34	29	14	6	33	31	5	3	44	44	13	0	21	27	2	8	31	36	2	8	31	36
15	2	42	41	24	1	41	37	5	6	28	22	10	10	23	20	23	0	40	33	5	5	32	35	13	1	33	30	2	10	46	44	3	0	32	29
15	3	29	26	24	2	24	20	5	7	52	49	11	1	36	38	20	5	31	26	5	6	52	52	13	3	41	40	3	0	32	29	3	1	29	35
15	4	36	18	24	3	23	22	5	9	21	27	11	2	28	31	20	7	29	31	5	7	78	75	13	4	26	25	3	1	29	35	3	2	33	35
15	5	29	27	25	1	21	22	5	10	23	22	11	3	41	42	21	1	40	41	5	8	31	30	13	5	25	20	3	2	33	35	3	1	54	53
15	6	28	29					5	11	23	23	11	4	57	55	21	2	21	27	5	9	42	42	13	6	27	22	3	1	54	53	3	1	54	53
15	7	25	20					5	12	22	18	11	5	43	41	21	3	21	11	6	0	95	99	13	7	20	13	3	4	12	31	3	4	12	31
15	8	38	34					6	1	38	39	11	6	29	29	21	4	34	31	6	1	33	34	13	8	25	21	3	6	29	31	3	6	29	31
16	1	22	23	0	1	19	13	6	2	31	27	11	7	32	40	22	1	34	32	6	2	99	56	14	0	31	26	3	7	20	11	3	7	20	11
16	2	42	40	0	3	31	44	6	3	60	64	11	9	49	46	21	0	56	55	6	3	36	33	14	1	11	11	3	10	21	11	3	10	21	11
16	3	33	32	0	4	53	65	6	5	31	32	11	11	22	24	23	2	32	31	6	4	27	28	14	2	20	19	4	0	49	55	4	0	49	55
16	4	55	54	0	7	40	40	6	6	30	41	12	1	26	30	23	3	24	23	6	5	31	31	14	3	31	32	4	1	26	31	4	1	26	31
16	5	32	32	0	8	39	36	6	7	63	63	12	3	54	58	24	2	22	19	6	6	19	19	15	0	26	24	4	6	67	67	4	6	67	67
16	6	32	34	0	10	41	38	6	8	57	53	12	5	38	37					6	7	35	32	15	1	34	35	4	7	26	24	4	7	26	24
17	1	33	32	1	0	43	42	6	11	29	28	12	7	27	31					6	9	25	29	15	2	24	27	4	8	60	62	4	8	60	62
17	2	29	26	1	1	18	16	7	0	60	64	12	8	24	24					6	11	21	18	15	5	26	29	4	9	31	32	4	9	31	32
17	3	24	26	1	2	99	103	7	1	90	85	12	9	21	22					0	0	31	35	15	7	23	16	5	1	25	27	5	1	25	27
17	4	39	42	1	3	65	65	7	2	78	78	13	0	30	28					0	1	45	47	15	8	21	18	5	2	37	37	5	2	37	37
17	5	31	30	1	4	50	46	7	3	24	28	13	1	32	29					0	3	67	63	16	2	52	54	5	4	26	26	5	4	26	26
17	6	36	38	1	5	17	19	7	4	36	37	13	2	55	56					0	6	25	25	16	4	24	21	5	5	34	36	5	5	34	36
17	7	27	16	1	6	27	28	7	6	41	44	13	3	21	21					0	11	40	38	17	0	52	55	5	6	20	20	5	6	20	20
18	2	44	41	1	12	22	25	7	7	36	35	13	4	39	35					1	0	23	32	17	2	26	26	5	10	21	15	5	10	21	15
18	3	30	26	2	0	22	17	7	8	37	34	13	6	31	29					1	1	18	21	17	4	28	26	6	4	28	26	6	4	28	26
18	4	36	40	2	1	22	27	7	9	40	38	13	7	25	21					1	3	46	42	18	0	29	31	6	2	49	50	6	2	49	50
18	5	28	27	2	5	51	55	7	14	34	32	13	8	34	38					1	4	26	26	18	1	47	53	6	3	26	27	6	3	26	27
18	6	39	39	2	6	27	28	8	1	38	38	13	10	37	31					1	5	30	25	18	2	29	28	6	4	32	25	6	4	32	25
18	7	23	21	2	7	41	41	8	2	36	35	14	2	35	38					1	6	20	19	18	3	47	41	6	5	46	46	6	5	46	46
19	1	23	10	2	8	32	27	8	3	46	43	14	3	25	21					1	7	24	29	18	4	42	41	6	7	25	22	6	7	25	22
19	2	27	29	2	9	42	39	8	4	30	28	14	4	54	53					1	9	50	44	19	5	35	33	6	8	82	82	6	8	82	82
19	3	27	23	2	10	23	25	8	5	25	24	14	7	30	30					1	10	39	38	19	6	25	21	6	9	24	28	6	9	24	28
19	4	48	53	2	12	21	13	8	6	37	35	15	0	43	45					1	11	26	25	20	1	24	25	7	2	24	24	7	2	24	24
19	5	44	44	3	0	40	47	8	7	64	61	15	1	31	32					2	0	64	67	20	4	35	32	7	4	35	32	7	4	35	32
19	6	26	22	3	1	116	116	8	8	44	41	15	2	27	30					2	1	28	28	21	0	38	38	7	5	27	28	7	5	27	28
19	7	24	25	3	2	25	32	8	9	34	32	15	3	51	48					2	2	71	77	21	2	34	35	7	6	28	31	7	6	28	31
20	0	22	23	3	3	85	84	8	11	24	17	15	4	37	36					2	3	22	21	21	3	29	26	7	7	27	22	7	7	27	22
20	1	31	29	3	4	35	35	9	0	82	90	16	1	25	25					2	4	32	28	22	4	24	20	8	1	66	66	8	1	66	66
20	2	21	12	3	5	17	19	9	1	43	48	16	5	40	41					2	5	23	22	22	5	21	21	8	2	28	31	8	2	28	31
20	3	44	45	3	6	28	29	9	2	17	15	16	6	22	23					2	7	19	13	22	6	14	14	8	3	47	47	8	3	47	47
20	4	41	41	3	8	19	20	9	3	46	43	16	7	24	19					2	8	19	13	10	2	50	50	8	4	32	31	8	4	32	31
20	5	22	13	3	11	40	37	9	4	29	25	16	9	30	29					2	10	34	31	10	3	36	31	8	6	54	59	8	6	54	59
20	6	26	28	4	0	28	35	9	5	41	46	17	1	32	30					3	1	35	34	10	4	26	23	8	7	28	26	8	7	28	26
20	7	23	22	4	2	42	41	9	6	24	26	17	3	15	34					3	2	26	23	10	5	54	55	8	8	33	35	8	8	33	35
21	1	38	18	4	3	30	27	9	7	32	32	17	4	37	34					3	5	20	26	10	7	51	50	9	1	41	40	9	1	41	40
21	2	20	21	4	4	38	41	9	8	48	49	17	5	38	42					3	6	43	44	10	8	20	18	9	2	26	18	9	2	26	18
21	3	33	32	4	5	25	24	9	9	21	23	17	7	46	44					3	7	53	48	10	9	25	30	9	5	43	46	9	5	43	46
21	4	20	20	4	6	57	58	9	10	38	37	18	0	23	25					3	8	51	52	11	0	22	13	10	0	30	29	10	0	30	29
21	5	27	26	4	7	19	19	9	11	25	24	18	1	22	17					3	10	31	26	11	2	51	52	10	1	31	30	10	1	31	30
21	6	27	23	4	8	32	31	10	0	35	34	18	2	24	22					4	1	84	82	11	4	38	41	1	2	49	47	10	2	40	48
22	0	30	31	4	9	42	39	10	1	19	21	18	4	34	30					4	2	44	50	11	7	25	24	1	3	32	35	10	3	32	35
22	1	23	23	4	10	33	31	10	2	52	52	18	6	37	34					4	3	63	61	11	8	24	21	10	4	39	42	10	4	39	42
22	2	46	46	4	11	23	19	10	3	51	52	18	8	24	20	</																			

Table B. (concluded)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
12	0	29	32	4	1	24	22	0	6	28	27	5	1	25	24
12	2	42	46	4	2	31	31	1	6	43	39	5	2	37	37
12	1	31	31	4	6	32	32	1	1	27	23	6	0	27	28
12	4	25	17	4	7	41	35	1	2	51	45	7	1	34	32
12	7	21	18	4	8	21	19	1	3	41	33	8	1	21	18
13	1	25	23	5	0	42	37	1	4	33	33	8	2	29	28
13	2	20	31	5	2	34	37	1	7	30	37				
13	5	23	24	5	3	22	21	2	2	33	30				
14	1	23	20	5	4	44	43	3	1	55	50				
14	1	51	51	5	6	36	34	3	2	27	22				
14	3	21	22	5	7	49	49	3	3	26	23				
14	7	29	27	6	0	30	35	3	5	27	24				
15	1	26	26	6	1	33	31	3	6	48	47				
15	2	36	32	6	4	27	19	4	1	29	34				
15	3	24	23	6	6	47	43	4	3	37	38				
15	4	20	19	7	1	44	43	4	6	32	32				
16	0	60	60	7	2	27	25	5	0	41	43				
16	1	25	28	7	1	54	54	5	2	23	18				
16	2	28	24	7	5	24	29	5	5	35	30				
16	3	27	26	7	6	36	36	5	6	23	20				
16	5	22	17	7	7	21	23	6	2	53	51				
16	6	22	27	7	8	33	33	6	3	41	30				
17	1	26	31	8	1	29	31	6	4	24	28				
17	2	29	27	8	2	33	34	6	5	23	23				
17	1	35	35	8	5	26	29	7	6	36	33				
18	0	32	30	8	7	26	24	7	1	27	22				
18	1	32	33	9	0	43	37	7	2	22	21				
18	2	33	30	9	2	50	55	7	6	28	27				
19	2	35	43	9	3	30	30	8	1	24	23				
20	0	39	41	9	4	45	38	8	2	29	32				
20	1	27	28	9	7	35	32	8	3	36	36				
				10	0	20	26	8	4	25	29				
				10	1	21	16	9	0	28	25				
				10	2	23	23	9	1	31	31				
				10	3	29	24	9	2	23	16				
0	0	36	33	11	1	21	24	10	1	25	29				
0	1	31	29	11	2	33	34	10	2	25	20				
0	2	35	42	11	3	45	42	10	3	28	30				
0	6	48	46	11	4	25	29	11	0	21	16				
1	0	25	19	12	1	25	23	11	2	35	34				
1	1	23	24	12	2	25	23	12	2	35	31				
1	3	22	24	12	5	27	25	14	1	24	17				
1	5	20	25	13	0	24	25								
2	0	24	26	13	1	22	26								
2	1	35	32	13	3	26	26								
2	2	31	24	14	2	27	27								
2	5	31	36	15	1	31	32	0	0	26	27				
2	6	28	29	15	3	23	25	0	2	46	41				
2	7	39	43	16	0	20	15	0	3	27	29				
2	8	22	19	16	1	22	16	0	4	36	34				
3	2	25	27	17	0	40	38	1	1	25	22				
3	3	30	28	17	2	24	24	2	1	28	30				
3	5	23	23					2	3	37	31				
3	6	33	33					2	4	22	22				
3	7	34	41					3	1	21	17				
3	8	23	30	0	2	23	26	3	2	36	33				
4	0	23	19	1	3	20	13	4	3	25	21				

Table C. Observed (FO) and Calculated (FC) Structure Factors for $\text{Fe}_2(\text{DSALZ}) \cdot \text{C}_3\text{H}_6\text{O}$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	
M= 0				0	10	83	87	1	17	27	29	7	5	78	75	15	4	18	10	3	11	84	83	0	6	24	24	17	7	19	26	
0	2	182	222	8	12	41	45	2	1	69	43	7	7	33	30	15	5	53	57	3	19	22	20	0	8	58	63	18	3	20	25	
0	4	194	188	9	14	42	46	2	2	230	222	7	9	105	101	15	9	33	33	4	0	142	84	0	9	32	40	10	4	18	17	
0	6	6	31	9	1	66	68	2	3	62	117	7	10	19	21	16	1	18	16	4	1	135	113	0	10	45	66					
0	8	178	178	9	3	53	17	2	4	83	75	7	11	39	38	16	5	21	28	4	2	57	22	0	11	17	18			M= 3		
0	10	72	73	9	5	86	85	2	5	81	94	7	12	26	29	17	3	24	27	4	3	68	68	0	12	47	44					
0	12	47	50	9	7	59	59	2	6	62	61	7	13	58	60	17	5	30	38	4	4	52	14	0	14	21	17	0	1	51	59	
0	14	67	66	9	15	25	29	2	7	13	12	7	15	28	27	18	6	28	24	4	5	34	44	0	1	37	38	0	3	175	95	
1	3	121	261	10	2	19	21	2	8	75	76	0	2	30	22					4	6	41	27	0	2	14	6	0	5	229	179	
1	5	44	36	10	4	11	41	2	9	23	15	0	3	24	3			M= 2		4	7	23	31	0	3	54	58	0	7	49	51	
1	7	24	26	10	6	22	22	2	10	59	57	0	4	22	17					4	9	23	24	0	4	83	78	0	9	130	148	
1	9	22	29	10	9	16	11	2	12	51	53	0	5	57	46	0	0	287	346	4	10	25	25	0	5	26	33	0	11	32	40	
1	11	39	37	10	14	29	19	2	14	27	27	0	6	43	48	0	2	38	130	4	11	38	41	0	6	35	34	0	13	41	45	
1	13	22	29	10	12	39	40	2	16	38	32	0	8	24	21	0	4	220	222	4	12	23	38	0	7	47	49	0	15	31	34	
1	15	22	23	11	1	52	53	3	1	65	49	0	9	43	45	0	6	118	137	4	14	19	17	0	8	51	55	0	17	23	38	
2	0	166	212	11	3	43	47	3	2	202	157	0	10	35	39	0	8	167	143	4	15	51	56	0	9	16	13	1	2	89	76	
2	2	11	46	11	5	29	25	3	3	69	64	0	11	35	37	0	10	66	66	5	0	172	154	0	10	47	50	1	3	49	51	
2	4	92	130	11	7	43	41	3	4	41	23	0	12	33	35	0	12	36	36	5	1	142	121	0	11	24	23	1	4	23	37	
2	6	15	27	12	2	32	43	3	6	38	44	0	13	20	28	0	14	26	27	5	2	60	49	0	12	34	32	1	5	12	2	
2	8	101	101	12	4	24	18	3	7	17	4	0	1	91	96	1	0	315	348	5	3	53	50	0	14	27	23	1	6	59	67	
2	10	41	42	12	10	48	37	3	8	22	24	0	4	34	30	1	1	22	23	5	4	26	24	10	0	39	49	1	7	37	38	
3	1	15	44	13	1	28	25	3	9	52	54	0	5	89	89	1	2	19	15	5	8	14	18	10	1	40	46	1	8	88	74	
3	3	24	19	13	3	34	37	3	10	14	4	0	6	47	52	1	3	64	60	5	9	22	20	10	2	14	26	1	9	53	49	
3	5	95	89	13	7	21	24	3	11	15	16	0	8	16	18	1	4	195	143	5	11	66	64	10	3	26	22	1	12	47	46	
3	7	16	27	13	9	17	11	3	13	28	15	0	9	45	47	1	5	50	48	5	14	31	48	10	5	45	50	1	14	27	20	
3	11	80	73	13	11	32	34	3	14	25	24	0	9	13	27	24	1	7	52	45	6	1	84	84	10	9	17	17	1	16	19	21
3	15	44	46	14	2	24	23	3	16	24	23	10	1	26	32	1	8	182	88	6	2	74	88	10	11	25	24	2	1	244	258	
4	0	227	176	14	4	52	49	4	1	259	262	10	2	97	94	1	9	29	31	6	1	23	16	11	1	33	36	2	2	213	196	
4	2	23	27	14	6	19	16	4	2	159	148	10	4	19	14	1	10	44	41	6	5	47	52	11	3	34	32	2	3	137	76	
4	6	21	9	14	10	23	35	4	4	59	54	10	5	19	15	1	11	38	41	6	6	24	9	11	5	17	17	2	4	96	80	
4	1	16	43	15	1	19	17	4	5	38	59	10	6	73	74	1	12	16	14	6	7	42	58	11	6	24	23	2	5	101	76	
4	3	17	28	16	0	19	19	4	6	64	66	10	8	19	18	1	14	35	38	6	8	34	38	11	7	38	49	2	7	13	22	
4	5	67	54	16	4	68	57	4	7	16	17	10	9	23	23	2	0	124	75	6	9	28	25	12	1	34	38	2	8	67	69	
4	9	69	64	16	6	17	24	4	10	64	73	10	10	16	18	2	1	16	5	6	10	29	34	12	2	23	17	2	9	69	72	
4	13	7	28	17	8	22	27	5	1	141	123	10	12	26	27	2	2	41	70	6	11	21	18	12	3	37	37	2	10	69	65	
4	15	62	62	17	7	23	27	5	3	110	86	10	13	22	21	2	3	24	47	6	14	16	15	12	4	25	28	2	12	43	45	
5	13	27	31	18	4	17	17	5	4	17	17	11	1	14	8	2	4	86	29	7	0	188	178	12	6	21	24	2	13	38	39	
5	15	24	24	18	6	14	12	5	5	14	12	11	2	44	41	2	5	160	164	7	1	89	84	12	7	24	25	3	1	12	11	
5	0	93	34					5	6	61	54	11	6	21	19	2	6	37	35	7	2	16	18	12	11	25	28	3	2	61	77	
5	2	39	21					5	7	83	82	11	10	16	18	2	7	107	109	7	3	44	42	13	0	24	24	3	3	77	75	
5	4	47	65					5	9	30	25	11	12	24	27	2	8	43	32	7	4	117	118	13	1	20	19	3	4	4	5	
5	6	77	67	0	3	125	194	6	1	101	124	12	2	25	18	2	10	10	11	7	5	24	28	13	2	18	22	3	5	61	59	
5	8	52	49	0	9	45	45	6	2	135	125	12	4	48	48	2	11	25	28	7	6	48	35	13	4	34	31	3	6	148	126	
5	10	28	34	0	13	26	21	6	3	15	5	12	10	24	28	2	12	16	20	7	7	31	33	13	5	36	34	3	8	61	57	
5	14	24	30	0	15	20	20	6	4	20	12	12	12	18	13	2	13	30	30	7	8	47	48	13	6	28	16	3	10	55	34	
6	1	64	64	1	1	268	250	7	2	98	61	13	7	17	3	3	0	94	85	7	9	27	14	13	7	26	29	3	12	82	94	
6	3	53	46	1	3	25	13	8	5	15	12	13	3	17	14	3	1	88	94	7	10	55	54	13	10	29	28	3	13	14	44	
6	7	38	42	1	4	28	43	8	7	27	37	13	4	16	9	3	2	78	78	7	12	22	14	14	4	44	43	3	16	34	41	
6	9	38	42	1	6	98	82	8	8	26	38	13	5	33	34	3	3	82	86	7	14	24	24	15	0	34	36	4	1	94	71	
6	11	35	46	1	9	27	31	8	9	16	18	13	9	26	28	3	4	93	81	8	0	262	218	15	0	39	42	4	2	86	71	
6	13	224	189	1	7	46	47	8	10	88	94	13	10	29	25	3	5	28	27	8	1	58	45	15	0	22	16	4	3	71	82	
6	15	60	46	1	8	24	26	8	12	23	27	14	6	17	19	3	6	64	96	8	2	56	47	15	11	19						

Table C. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
4	3	23	24	11	1	24	26	2	15	23	27	8	2	33	39	0	11	39	44	5	9	71	76	12	1	21	23	2	10	57	68
4	9	17	9	11	2	103	100	3	0	123	99	8	3	28	25	0	13	43	41	5	10	37	34	12	2	68	68	2	14	33	40
4	10	54	60	11	5	22	21	3	2	62	30	8	6	18	8	1	1	156	150	5	11	16	22	12	3	22	25	3	0	54	47
4	11	20	15	11	9	21	39	3	5	95	81	9	0	144	153	1	2	69	55	9	16	22	24	12	9	46	54	3	1	94	72
5	1	145	149	11	6	21	28	3	6	75	69	9	1	38	30	1	3	85	62	6	1	39	49	12	6	32	35	3	2	94	36
5	2	129	126	11	0	17	19	3	7	64	50	9	2	42	43	1	4	56	55	6	3	51	44	12	9	27	23	3	3	152	163
5	5	34	45	11	10	34	37	3	9	15	15	9	4	104	109	1	5	122	119	6	9	110	97	12	10	29	26	3	4	52	41
5	8	25	30	11	12	17	17	4	0	65	63	9	5	17	14	1	5	44	44	6	6	72	74	13	1	69	69	3	5	13	14
5	10	57	52	11	14	23	19	4	1	44	35	9	6	23	24	1	9	65	57	5	7	43	35	13	2	22	24	3	6	17	27
5	11	35	32	12	1	33	39	4	2	33	9	9	7	26	27	1	10	42	42	6	8	20	12	13	3	16	12	3	7	111	100
5	14	31	36	12	5	40	33	4	3	105	91	9	8	60	53	1	11	16	14	6	9	38	42	13	4	23	23	3	9	15	16
5	16	31	35	12	9	22	31	4	4	13	41	9	10	63	62	1	12	20	23	6	10	21	24	13	5	19	10	3	11	69	69
6	1	121	97	13	2	17	16	4	6	62	75	9	12	31	33	1	13	22	21	6	13	32	29	13	9	20	20	3	15	26	29
6	2	90	95	13	6	20	24	4	7	100	106	9	14	25	30	1	14	23	23	7	1	61	65	14	1	25	17	4	0	136	120
6	3	71	76	13	10	22	22	4	8	25	34	10	1	59	56	2	1	31	10	7	2	44	36	14	5	20	27	4	1	42	50
6	5	73	73	14	1	39	47	4	9	10	22	10	2	15	4	2	2	101	100	7	3	15	14	15	1	27	31	4	3	47	46
6	6	27	31	14	3	19	14	4	11	70	66	10	3	01	00	2	3	163	160	7	4	56	56	15	2	21	23	4	5	35	31
6	8	41	47	14	5	35	36	4	15	39	43	10	4	48	45	2	4	44	34	7	5	76	73	15	7	20	16	4	6	27	40
6	9	53	47	14	9	32	29	5	1	25	14	10	5	37	43	2	5	40	105	7	6	25	23	15	9	24	25	4	7	43	47
6	10	34	31	15	4	16	8	5	1	23	7	10	6	32	35	2	6	44	37	7	7	16	22	16	1	42	42	4	8	15	1
6	13	49	49	15	1	30	42	5	4	51	46	10	7	46	47	2	7	52	45	7	8	31	28	16	5	20	19	4	9	25	26
7	1	17	29	16	3	24	17	5	1	25	14	11	1	33	39	2	10	24	23	7	9	61	64	16	7	21	21	4	10	17	22
7	2	60	63	16	5	32	32	5	5	46	35	11	1	31	36	2	12	25	25	7	10	13	25	16	7	21	21	4	11	38	35
7	4	44	41	16	7	17	14	5	6	110	108	11	4	17	20	2	13	22	26	7	13	21	22	17	2	23	25	5	0	30	39
7	5	69	64	16	9	20	22	9	8	27	20	11	6	32	20	2	14	26	31	9	1	22	26					5	1	45	51
7	8	19	21	17	2	14	23	9	10	21	10	12	0	66	67	3	1	16	7	0	2	23	20					5	3	27	26
7	9	23	33					5	14	34	31	12	1	44	49	3	2	69	70	0	3	20	19	0	0	10	22	5	4	36	33
7	10	20	29					6	0	113	124	12	3	22	17	3	3	75	97	0	5	96	87	0	2	21	31	5	5	92	84
8	1	102	61	0	0	171	130	6	1	91	93	12	5	36	34	3	4	22	22	0	7	24	32	0	4	135	111	5	6	24	14
8	2	70	55	0	2	136	66	6	2	23	37	12	7	37	39	3	5	110	97	0	8	15	4	0	6	55	47	5	7	62	74
8	3	56	60	0	4	57	76	6	3	45	51	12	9	16	15	3	6	94	93	0	9	51	95	0	8	77	89	5	8	10	22
8	4	83	92	0	5	45	38	6	5	89	70	12	9	19	15	3	7	49	42	0	10	42	43	0	10	22	27	5	9	20	33
8	5	123	129	0	5	22	40	6	6	15	23	12	11	27	26	3	8	92	51	0	13	37	42	0	12	40	32	5	10	16	12
8	6	23	15	0	12	21	16	6	7	54	49	13	0	20	21	3	9	41	20	9	1	72	70	0	14	26	22	5	11	34	44
8	8	21	25	1	0	230	142	6	8	37	37	13	2	25	24	4	10	74	73	9	2	29	31	0	16	21	30	5	14	10	11
8	9	60	79	1	1	69	31	6	9	47	54	13	4	44	40	3	12	16	15	9	3	10	13	1	0	80	66	5	15	27	29
8	10	23	27	1	2	173	150	6	10	40	40	13	8	22	24	3	14	24	25	9	4	35	39	1	1	33	16	6	0	135	116
8	12	20	21	1	3	41	40	6	13	21	10	13	10	26	24	4	2	44	44	9	5	50	46	1	2	130	104	6	1	50	43
8	13	45	40	1	4	135	140	6	15	20	23	13	12	17	10	4	3	31	10	9	6	31	32	1	3	54	53	6	2	14	9
9	1	73	70	1	5	12	5	7	0	73	79	14	9	40	91	4	4	23	12	9	9	20	32	1	4	64	53	6	4	40	47
9	2	62	61	1	6	147	124	7	1	32	24	14	3	16	14	4	5	46	34	9	12	20	20	1	5	10	16	6	6	51	60
9	4	14	8	1	8	105	112	7	2	16	32	15	0	49	56	4	6	155	153	9	13	20	20	1	6	84	76	6	7	15	19
9	5	34	35	1	9	19	16	7	3	19	16	15	2	24	27	4	7	42	42	10	1	20	20	1	7	43	44	6	8	46	41
9	7	37	42	1	10	59	64	7	4	130	129	15	4	35	35	4	9	13	22	10	2	60	50	1	8	39	35	6	10	59	55
9	8	25	20	1	12	54	47	7	5	24	32	17	0	37	42	4	11	21	12	10	5	10	11	1	11	30	25	6	14	12	37
9	12	21	19	1	14	35	40	7	6	65	69	17	4	30	29	4	12	34	42	10	7	35	36	1	12	22	35	7	0	17	7
9	14	19	22	2	9	79	195	7	8	64	61	18	3	22	24	4	14	36	34	10	9	21	32	2	0	76	67	7	2	13	22
10	1	46	40	2	3	154	115	7	9	27	27					4	16	21	26	10	10	21	22	2	1	14	13	7	4	39	36
10	2	30	41	2	4	103	127	7	10	20	10					5	1	64	91	11	2	13	95	2	2	169	85	7	5	69	61
10	3	52	53	2	5	51	30	7	11	19	13					5	2	90	97	11	3	47	51	2	3	122	124	7	7	25	23
10	4	17	23	2	7	11	91	7	12	44	40	0	1	43	30	5	3	13	30	11	5	25	10	2	4	154	132	7	9	20	10
10	5	51	54	2	8	19	10	7	13	23	29	0	3	76	95	5	4	30	24	11	6	02	02	2	5	62	60	7	11	20	25
10	6	91	50	2	10	44	41	7	14	27	20	0	5	210	222	5	5	01	53	11	8	20	17	2	6	70	66	7	12	22	20
10	7	29	25	2	11	91	93	8	0	92	99	0	6	27	49	5	6	00	40	11	10	26	30	2	7	60	56	8	0	93	93
10	9	39	35	2	14	29	30	8	1	44	41	0	8	02	71	5	6	44	61	11	12	29	20	2	8	50	60	8	2	31	23

Table C. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
5	3	23	26		M= 7			5	1	63	65	15	3	25	23	4	11	25	19	10	7	22	21	2	12	34	36	4	2	44	40				
4	4	35	37					6	2	42	34	15	5	26	27	4	15	14	15	10	12	20	17	2	13	33	30	4	3	35	35				
7	5	50	52	5	1	22	30	6	5	37	26	15	6	28	26	5	8	81	77	11	1	61	65	3	1	13	13	9	4	15	2				
8	7	40	34	8	3	35	32	6	6	56	59	15	9	31	31	5	1	89	79	11	2	16	18	3	2	24	34	9	5	55	53				
6	5	63	51	8	5	36	33	6	8	37	34	17	1	29	38	5	3	61	55	11	3	67	67	3	3	49	56	9	7	24	29				
9	10	50	43	8	7	14	27	6	9	24	14	17	5	18	19	5	4	94	53	11	7	28	26	3	4	34	36	9	8	33	38				
6	12	23	29	8	9	17	2	6	12	22	19	18	2	24	30	5	5	88	60	11	9	19	26	3	5	14	11	9	9	20	16				
9	14	22	21	1	1	175	162	7	1	49	48					5	6	37	36	11	11	44	46	3	6	11	91	9	10	14	20				
9	1	13	16	1	2	57	57	7	2	83	79	M= 8				5	7	72	77	12	0	52	46	3	8	19	22	9	13	22	16				
9	2	19	18	1	3	94	101	7	3	44	43	0	0	92	103	5	9	16	17	12	2	24	22	3	10	18	34	10	1	16	19				
9	3	29	26	1	4	51	47	7	5	99	100	0	4	180	98	5	10	17	21	12	11	22	21	3	12	39	41	10	2	93	91				
9	4	57	57	1	5	262	186	7	6	44	41	0	5	21	22	5	11	34	35	13	1	21	23	4	1	45	39	10	8	10	25				
9	6	34	31	1	6	15	7	7	9	92	83	0	6	63	55	5	15	23	21	13	2	16	27	4	2	81	84	10	9	70	22				
9	7	31	29	1	7	34	39	7	10	25	25	0	8	32	23	6	0	86	43	13	5	46	24	4	3	29	30	10	10	38	29				
9	9	16	15	1	9	11	16	7	13	36	36	0	10	32	23	6	2	16	1	13	6	23	32	4	4	26	27	11	1	32	30				
9	17	39	44	1	13	31	31	8	2	17	12	0	12	23	26	6	3	16	1	13	7	29	32	4	6	84	60	11	2	21	20				
9	11	47	37	2	2	42	73	8	3	29	32	0	14	37	40	6	3	21	23	13	7	29	32	4	6	84	60	11	2	21	20				
9	12	20	14	2	5	55	52	9	9	25	25	0	16	24	24	6	4	84	77	14	0	37	39	4	8	22	23	11	6	20	17				
10	8	43	45	2	4	63	63	0	10	30	35	1	0	68	44	6	6	32	22	14	3	27	22	4	12	40	39	11	10	31	29				
10	2	19	22	2	5	17	21	0	12	19	19	1	2	93	93	6	9	70	79	14	4	39	47	5	1	33	47	12	1	43	42				
10	1	40	41	2	6	79	61	6	14	21	16	1	3	82	74	6	9	20	14	14	6	20	21	5	2	141	137	12	2	26	29				
10	4	63	64	2	9	23	31	9	1	44	44	1	4	152	145	6	10	28	38	15	8	40	40	5	3	26	20	12	7	17	10				
10	5	21	19	2	10	35	40	9	2	22	20	1	5	42	39	6	11	22	29	15	4	26	26	5	4	57	56	13	1	21	21				
10	7	44	46	2	12	32	38	9	3	49	53	1	7	37	37	6	12	21	16	15	6	26	25	5	6	85	83	13	2	57	59				
10	11	29	27	2	14	33	34	9	5	81	85	1	9	43	35	6	14	26	26	16	0	26	24	5	9	19	28	13	6	31	33				
10	13	21	23	3	1	16	21	9	6	25	28	1	10	26	20	7	8	48	49	16	3	23	22	5	10	33	36	13	10	29	29				
11	1	44	45	3	2	53	46	9	9	51	47	1	11	24	24	7	1	32	29	16	4	24	23	5	11	17	19	14	1	46	35				
11	1	55	54	3	3	16	18	9	13	48	42	2	0	20	20	7	2	32	38	18	8	22	24	5	12	27	28	14	3	39	44				
11	5	19	21	3	4	44	38	10	2	82	82	2	2	15	22	7	4	32	27	19	14	25	23	5	14	25	23	14	5	61	65				
11	7	44	44	3	5	15	2	10	4	16	16	2	3	19	22	7	6	82	68					6	1	66	63	14	6	19	14				
11	9	15	17	3	6	10	9	10	6	21	22	2	4	112	103	7	7	29	34					6	2	48	41	14	9	22	30				
11	11	39	36	3	7	21	25	10	10	51	53	2	6	42	51	7	8	31	33					6	3	88	76	15	2	25	27				
12	9	37	35	3	9	21	11	10	12	24	28	2	7	44	42	7	9	21	19					6	4	19	28								
12	1	20	21	3	9	24	32	11	2	48	45	2	8	46	39	7	10	35	37					6	5	111	117								
12	2	32	38	3	13	21	21	11	3	23	29	2	9	22	24	7	12	22	21					6	7	45	40								
12	5	16	7	3	14	18	16	11	4	24	23	2	10	26	19	7	14	23	27					6	8	19	22								
12	6	25	21	4	1	43	39	12	1	29	40	2	11	28	33	8	0	67	78					6	9	48	45								
12	7	25	19	4	2	79	78	12	2	64	66	2	12	19	29	8	4	81	79					6	13	27	30								
12	9	19	16	4	4	59	54	12	3	16	24	2	14	30	37	8	6	31	38					6	14	21	17								
12	10	22	21	4	5	19	24	12	4	20	24	2	16	21	33	8	7	22	25					7	1	35	42								
13	1	27	32	4	6	125	117	12	5	17	17	3	1	61	65	8	8	31	31					7	3	34	27								
13	1	17	18	4	7	22	16	12	6	35	36	3	2	31	36	8	10	36	39					7	5	20	17								
13	4	39	44	4	11	77	76	12	8	24	21	3	3	124	119	8	12	29	28					7	7	16	23								
13	5	25	29	4	12	58	57	12	10	40	37	3	4	33	41	9	8	19	24					7	8	55	56								
13	7	21	25	4	14	24	24	12	12	20	18	3	5	52	54	9	1	31	32					7	9	19	22								
13	11	17	23	4	16	24	39	13	1	39	37	5	7	76	76	9	3	44	48					7	10	19	19								
14	0	53	62	5	1	57	55	13	2	31	40	3	11	65	67	9	4	28	22					7	13	21	30								
14	4	26	27	5	2	52	51	13	5	39	34	3	15	28	21	9	6	10	13					7	15	17	19								
14	8	37	34	5	3	20	19	13	7	17	6	4	0	88	78	9	7	21	15					7	17	17	19								
14	10	27	32	5	5	42	46	13	9	34	34	4	1	32	20	9	8	38	28					7	19	17	19								
15	2	17	17	5	6	58	47	14	1	27	34	4	2	35	2	9	11	35	35					7	21	16	19								
15	8	59	65	5	7	18	12	14	3	17	17	4	3	41	36	10	0	34	25					7	23	14	19								
16	4	35	33	5	8	36	35	14	5	24	23	6	4	49	39	10	1	26	26					7	25	14	19								
16	8	22	23	5	9	47	46	15	6	27	26	6	7	33	39	10	2	16	15					7	27	14	19								
16	8	27	31	5	13	28	26	15	1	23	21	4	8	42	41	10																			

Table C. (continued)

K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	
2	6	21	20	9	4	48	34	3	3	13	2	11	4	17	16	4	0	25	14	11	2	34	39	4	12	56	64	1	2	36	36	1	2	36	36	
2	7	73	65	10	0	29	34	3	4	51	53	11	6	44	45	4	1	77	77	11	3	23	34	5	1	47	39	1	3	34	31	1	3	34	31	
2	11	55	55	10	1	44	46	1	5	37	40	11	7	19	21	4	3	66	45	11	9	27	29	5	2	33	32	1	4	35	41	1	4	35	41	
2	13	14	27	10	3	32	35	3	6	65	65	11	8	37	36	4	4	27	32	11	7	10	14	5	3	55	59	1	5	27	23	1	5	27	23	
2	15	21	23	10	5	34	34	3	8	22	17	12	1	16	19	4	5	31	30	12	1	39	40	5	4	20	30	1	6	16	19	1	6	16	19	
7	0	92	94	10	7	38	34	3	9	20	22	12	2	20	24	4	7	42	37	12	3	36	34	5	5	63	66	2	0	87	73	2	0	87	73	
3	1	40	35	11	8	36	31	3	10	21	21	12	3	32	40	4	8	18	18	12	7	37	44	5	6	35	32	2	4	79	87	2	4	79	87	
3	2	88	73	11	2	30	26	3	12	52	51	12	9	21	23	4	11	32	39	13	0	26	22	5	9	26	32	2	5	19	21	2	5	19	21	
3	3	31	29	11	6	21	18	4	1	19	7	12	6	18	14	5	0	68	76	13	6	16	11	5	11	20	22	2	7	17	24	2	7	17	24	
3	4	41	71	11	7	26	34	4	2	39	38	13	2	37	37	5	1	29	50	13	7	24	29	5	12	22	24	2	8	59	59	2	8	59	59	
3	5	31	28	11	4	24	24	4	3	61	53	13	5	30	36	5	2	21	10	14	0	24	29	6	2	32	31	2	9	23	15	2	9	23	15	
3	6	21	19	12	1	43	45	4	7	24	19	13	6	30	29	5	3	95	56	14	3	19	22	6	4	23	26	2	10	27	31	2	10	27	31	
3	8	19	26	12	3	44	44	4	10	32	38	13	8	28	22	5	4	45	43	14	4	24	23	6	6	41	41	2	12	20	23	2	12	20	23	
3	12	24	23	12	5	28	27	5	1	15	25	14	1	29	25	5	5	35	31	14	6	20	19	6	10	24	29	3	0	26	17	3	0	26	17	
4	1	98	85	12	6	17	18	5	2	101	108	14	3	29	32	5	6	27	25	15	8	22	30	7	1	42	40	3	1	75	76	3	1	75	76	
4	2	44	42	12	7	42	47	5	3	16	3	14	5	30	35	5	7	34	37	15	4	21	26	7	3	64	68	3	2	52	57	3	2	52	57	
4	3	89	87	12	11	32	31	5	4	43	49	15	5	19	17	5	11	38	40	16	8	26	23	7	4	22	24	3	3	84	83	3	3	84	83	
4	4	30	20	13	8	21	18	5	5	20	23	16	1	35	20	5	13	28	16	16	0	26	23	7	5	42	41	3	5	51	50	3	5	51	50	
4	5	41	46	13	1	17	14	5	6	81	88	16	5	19	19	6	0	62	54	16	0	26	23	7	7	25	28	3	6	34	28	3	6	34	28	
4	7	59	97	13	2	26	23	5	9	17	19	16	5	19	19	6	1	27	26	16	0	26	23	7	8	16	17	3	7	71	69	3	7	71	69	
4	9	30	33	13	4	50	52	5	10	35	34	16	5	35	34	6	3	21	23	16	1	23	48	7	9	51	52	3	11	51	52	3	11	51	52	
4	11	47	52	13	6	33	35	5	12	33	40	16	5	35	40	6	4	73	76	16	3	16	26	7	10	16	11	4	0	22	36	4	0	22	36	
4	15	35	38	14	8	17	15	5	13	17	15	16	6	4	33	28	6	6	33	28	16	5	25	33	7	12	19	13	4	1	29	29	4	1	29	29
5	0	65	57	14	6	20	22	5	14	24	21	16	6	24	21	6	7	61	57	16	0	34	36	7	1	24	19	4	4	23	15	4	4	23	15	
5	1	31	30	15	8	52	56	6	1	37	42	16	6	24	23	6	9	11	26	16	0	42	40	8	2	30	31	4	5	22	23	4	5	22	23	
5	2	59	70	15	4	39	42	6	2	32	32	16	8	10	22	31	6	10	36	32	16	13	16	18	8	4	24	23	5	0	20	22	5	0	20	22
5	3	18	16	15	6	19	21	6	3	59	56	16	14	19	19	6	11	20	26	16	1	1	19	19	8	7	12	16	5	1	53	54	5	1	53	54
5	4	40	44	16	1	19	19	6	5	66	53	1	8	51	41	6	13	22	25	1	2	21	34	8	9	18	19	5	3	62	68	5	3	62	68	
5	6	33	41	16	3	23	26	6	8	37	37	1	1	28	17	7	0	62	64	7	3	49	40	9	1	42	38	5	4	56	59	5	4	56	59	
5	7	16	13	16	9	21	26	6	9	21	26	1	2	37	21	7	2	15	12	7	5	53	49	9	5	23	23	5	5	30	29	5	5	30	29	
5	9	19	23	16	13	32	33	6	13	32	33	1	4	62	40	7	4	67	63	7	6	42	40	9	6	44	40	5	6	21	21	5	6	21	21	
6	0	23	21	16	1	22	32	7	1	22	32	1	5	34	32	7	5	23	21	7	7	24	31	9	9	33	30	5	7	54	54	5	7	54	54	
6	1	50	48	16	1	98	92	7	2	15	13	1	8	31	31	7	6	25	21	7	8	19	17	10	1	19	11	5	11	47	51	5	11	47	51	
6	3	92	19	16	3	127	134	7	3	25	23	1	11	16	10	7	7	23	13	7	9	26	22	10	2	34	37	6	8	78	92	6	8	78	92	
6	4	15	0	16	5	98	108	7	5	48	43	1	14	26	29	7	8	33	33	7	8	33	33	1	13	32	33	6	3	36	31	6	3	36	31	
6	6	16	13	16	7	23	14	7	6	45	44	2	0	66	99	7	10	37	35	7	10	37	35	2	2	85	83	6	4	59	56	6	4	59	56	
6	7	30	30	16	9	54	55	7	9	20	20	2	1	23	29	8	0	40	34	8	0	40	34	2	3	20	26	6	5	26	25	6	5	26	25	
6	9	18	4	16	13	52	53	8	1	63	63	2	3	76	81	8	1	29	30	8	1	29	30	2	4	54	52	11	2	19	17	6	8	54	57	
6	9	23	19	16	15	22	25	8	3	62	56	2	4	73	69	8	3	21	19	8	3	21	19	2	5	16	17	11	8	25	21	6	9	22	19	
6	11	36	33	16	1	14	1	8	5	68	69	2	5	26	26	8	4	34	43	8	4	34	43	2	6	25	25	12	2	39	41	6	10	36	38	
7	0	115	107	16	1	2	78	66	8	6	15	17	2	7	29	23	8	7	26	25	8	7	26	25	2	10	33	32	12	6	33	40	6	12	32	38
7	2	16	5	16	1	3	25	33	8	7	38	32	2	8	41	39	8	9	26	25	8	9	26	25	2	12	19	21	12	8	19	24	7	2	22	17
7	4	185	113	16	4	16	16	8	9	54	58	2	10	17	22	8	0	29	28	8	0	29	28	3	1	18	24	13	1	26	27	6	0	54	56	
7	6	65	71	16	5	26	38	9	13	33	35	2	11	29	25	8	9	21	24	8	9	21	24	3	2	53	47	13	2	20	21	8	2	26	31	
7	7	49	52	16	6	49	49	9	1	19	22	2	12	28	22	9	1	23	23	9	1	23	23	3	3	10	17	14	6	23	21	8	3	15	11	
7	8	36	32	16	9	17	13	9	2	64	64	2	14	19	17	9	4	27	26	9	4	27	26	3	4	23	23	15	1	31	30	8	4	21	14	
7	10	35	35	16	1	9	19	13	9	3	15	13	3	0	36	19	9	6	26	23	9	6	26	23	3	5	36	36	15	3	21	18	8	5	22	18
7	12	34	34	16	12	24	27	9	5	16	20	3	1	63	68	9	12	19	22	9	12	19	22	3	6	54	56	15	6	21	19	8	6	21	19	
7	14	39	37	16	1	61	45	9	6	34	38	3	2	33	27	10	0	91	50	10	0	91	50	3	9	49	55	15	7	17	19	8	7	17	19	
8	0	21	23	16	2	38	27	9	7	22	24	3	3	52	47	10	1	22	19	10	1	22	19	3	11	16	21</									

Table C. (concluded)

	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
11	3	47	49	7	5	31	32	4	1	55	59	2	1	31	22	4	5	39	39	H= 20	3	1	24	32
11	7	42	45	7	5	15	17	4	2	31	21	2	3	21	24	4	7	73	76		7	3	26	31
12	9	27	29	7	5	15	15	4	3	79	82	2	5	11	22	5	0	33	33	0	0	63	64	
13	1	21	20	7	5	16	17	4	3	15	15	5	2	41	25	5	2	11	25	0	0	25	36	
13	1	19	19	7	7	16	15	4	5	25	24	2	9	29	35	5	0	4	24	0	0	3	31	
13	3	25	25	0	1	17	13	4	7	65	60	3	2	41	30	5	5	22	20	1	2	22	30	
13	7	31	30	0	5	24	26	4	11	25	26	3	3	10	10	0	7	26	29	1	4	23	23	
14	0	40	39	0	9	21	22	5	0	53	61	3	4	25	23	7	0	26	26	1	7	19	22	
14	4	23	24	9	1	17	19	5	1	32	32	3	4	53	54	7	3	29	24	2	0	49	49	
				9	2	19	22	5	2	23	23	3	0	61	65	7	4	26	31	2	1	20	19	
				9	3	26	26	5	3	32	40	3	10	25	21	7	0	32	31	2	0	25	29	
				9	5	25	26	5	4	35	37	4	2	30	26	0	0	29	30	3	1	41	44	
				10	2	30	34	5	5	19	16	4	3	34	40	0	6	20	25	3	3	42	49	
				10	4	19	20	5	7	35	45	4	4	18	19	0	7	21	13	3	9	17	11	
				10	6	24	24	5	0	20	20	4	6	19	22	9	0	29	20	3	7	41	42	
				10	0	24	20	5	11	24	27	5	1	17	19	9	4	31	39	4	1	20	27	
				11	2	24	23	6	0	40	46	5	2	74	74	10	1	19	21	4	3	23	15	
				11	3	27	23	6	2	27	20	5	6	50	40	10	3	27	26	4	5	30	32	
				11	6	43	20	6	3	29	31	5	0	45	46	12	1	24	21	4	7	19	23	
				12	2	45	49	6	0	30	42	5	10	22	19					5	1	21	21	
				12	6	31	20	7	0	30	37	6	1	46	52					5	2	19	23	
				13	1	24	25	7	2	19	22	6	5	50	48					5	3	38	42	
				13	5	19	10	7	4	39	40	6	9	35	39	0	3	57	56	5	4	22	29	
								7	6	29	29	7	4	17	13	0	5	24	29	5	5	10	20	
								7	6	27	26	8	3	37	37	1	1	52	53	5	7	35	40	
								8	10	19	17	8	5	35	36	1	2	23	27	6	0	36	33	
								8	5	45	41	0	9	30	33	1	3	36	32	6	4	29	31	
								8	5	10	10	9	6	34	34	1	9	30	32	7	0	27	10	
								8	6	22	20	10	3	19	23	2	2	44	44	4	0	27	22	
								9	0	23	23	11	2	43	41	2	3	29	26	0	4	22	22	
								9	4	39	35	11	4	10	21	2	4	34	30					
								9	7	24	20	11	6	30	39	2	5	34	35					
								9	0	22	21	2	6	20	26	2	6	20	26					
								10	1	10	17					2	0	30	29	0	1	20	21	
								10	3	29	31					2	9	22	22	1	1	37	30	
								10	4	31	37	0	0	46	49	3	1	26	23	1	3	25	29	
								10	7	15	14	0	2	41	49	3	2	44	49	1	5	22	20	
								11	1	10	26	0	6	23	25	3	6	30	41	1	7	19	21	
								11	2	10	19	0	0	18	16	3	0	31	30	2	2	53	57	
								11	3	29	31	1	0	25	25	4	6	19	10	2	6	33	36	
								11	7	26	20	1	3	17	19	4	0	31	30	4	2	49	52	
								12	0	10	21	1	4	39	41	5	2	43	41	4	6	29	24	
								12	1	20	20	1	5	24	23	5	4	19	14	5	4	21	16	
								12	3	32	36	1	6	30	31	5	6	37	40	6	2	27	35	
								13	0	22	20	1	0	27	29	5	8	26	20	6	3	10	10	
								13	3	19	16	2	1	10	17	6	1	20	25	7	1	30	34	
												2	2	10	15	6	2	46	47	7	3	24	24	
												3	3	42	44	6	3	39	40					
												2	7	40	40	6	5	20	22					
												3	0	33	29	6	6	24	25					
												3	2	20	26	7	1	33	31	0	0	49	49	
												3	4	20	20	7	9	27	31	0	4	26	29	
												3	7	21	26	9	2	19	17	1	0	20	31	
												4	1	49	49	9	3	26	22	1	3	23	19	
												4	2	36	30	10	2	27	29	2	0	31	34	
												4	3	01	04					2	1	20	20	

Table D. Observed (FO) and Calculated (FC) Structure Factors for $[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	
H=-18				3	0	75	76	3	9	17	15	1	10	42	43	6	5	22	20	2	2	48	49	3	8	41	41	6	5	12	11	
				3	2	40	38	3	10	37	37	1	11	18	17	6	6	29	29	2	3	41	39	3	10	78	78	6	6	33	30	
0	0	39	39	3	3	24	24	5	0	21	23	3	0	16	16	6	8	50	49	2	4	41	41	3	12	18	23	6	8	44	45	
0	2	54	53	3	5	14	11	5	1	17	17	3	1	14	12	8	0	57	58	2	5	15	10	5	0	49	51	6	9	13	14	
0	4	70	69	3	6	55	54	5	2	24	24	3	2	40	40	8	2	32	31	2	6	52	52	5	1	28	31	8	0	00	05	
0	6	14	12	3	8	54	53	5	3	37	36	3	3	16	19	8	3	15	14	2	7	13	13	5	2	75	75	8	2	76	74	
2	1	13	13	5	0	45	44	5	4	40	37	3	4	54	55	8	4	17	17	2	8	55	55	5	3	45	46	8	3	16	16	
2	2	35	35	5	1	32	32	5	5	16	16	3	6	22	21	8	4	17	17	2	9	22	21	5	4	55	56	8	4	21	20	
2	3	10	18	5	2	26	25	5	6	32	30	3	8	65	63	H=-9				2	10	45	46	5	5	47	44	8	6	34	29	
2	5	10	15	5	4	26	25	5	7	27	27	3	10	33	34	2	12	33	32	4	0	112	119	5	6	35	32	H=-5				
2	6	22	22	5	5	15	16	5	8	14	22	1	0	54	55	1	1	11	12	4	0	162	104	5	7	35	35	H=-5				
				5	6	42	42	7	4	29	29	5	2	60	59	1	2	133	135	4	2	162	104	5	8	35	34	H=-5				
H=-17												5	3	45	43	1	3	34	32	4	3	44	45	5	10	25	25	1	0	29	41	
1	0	55	57	H=-14				H=-12				5	4	32	32	1	4	55	55	4	4	4	11	4	6	48	51	7	2	15	13	
1	1	53	52	0	0	27	25	0	0	18	17	5	6	29	27	1	5	43	43	4	7	16	16	7	3	14	12	1	3	73	04	
1	2	39	40	0	2	13	12	0	2	121	120	5	7	17	14	1	7	24	22	4	8	66	65	7	5	16	16	1	4	197	184	
1	6	36	30	0	4	52	51	0	4	102	103	5	8	35	35	1	8	33	33	4	9	13	12	7	6	55	55	1	5	78	76	
1	7	16	14	0	6	95	97	0	6	15	18	5	9	15	17	1	9	22	25	4	10	16	16	7	7	17	18	1	6	87	85	
1	8	38	28	0	8	36	35	0	8	53	53	7	0	24	23	1	10	62	63	6	0	32	35	6	0	49	49	1	7	29	30	
3	0	22	22	0	10	27	26	0	10	62	62	7	1	12	11	1	11	24	25	6	1	41	41	6	1	41	41	1	8	32	31	
3	1	17	13	2	0	30	29	2	4	26	28	7	2	15	10	1	12	14	14	6	2	24	22	H=-6				1	9	14	12	
3	2	46	47	2	1	35	35	2	1	39	38	7	4	48	47	3	0	74	76	6	3	52	51	6	4	43	42	1	10	31	30	
3	4	36	35	2	2	41	43	2	2	49	50	7	6	46	46	3	1	11	18	6	4	43	42	6	0	136	132	1	11	31	30	
3	7	14	12	2	3	51	51	2	4	67	69	H=-10				3	2	15	16	6	5	26	25	6	0	2	146	152	1	12	29	29
H=-16				2	4	36	35	2	5	36	36	4	0	125	129	3	3	24	22	6	6	22	21	6	4	34	36	3	0	110	110	
				2	5	21	21	2	6	39	40	4	0	125	129	3	4	83	84	6	7	20	20	6	6	110	112	3	1	71	01	
0	0	61	62	2	6	12	16	2	8	18	18	4	2	51	47	3	5	16	16	6	8	22	22	6	8	22	22	2	2	33	32	
0	2	77	77	2	8	41	41	2	10	29	29	4	4	41	41	3	6	74	72	6	9	33	32	6	0	33	32	2	3	46	45	
0	6	14	12	2	10	37	33	4	4	65	66	4	6	24	25	3	8	36	34	8	0	33	32	6	1	31	33	3	4	26	25	
0	8	47	49	4	0	44	43	4	1	27	30	4	8	47	48	3	10	37	36	8	4	47	46	6	0	50	52	3	5	18	18	
2	0	37	38	4	2	66	64	4	2	13	13	4	10	25	26	3	10	25	26	8	4	47	46	6	1	15	15	3	6	110	110	
2	2	28	28	4	4	37	35	4	4	40	40	4	12	46	44	5	1	41	42	8	5	47	46	6	2	31	25	3	7	20	17	
2	3	31	34	4	5	13	14	4	5	26	26	4	14	45	46	5	2	73	74	8	6	88	87	6	3	92	95	3	8	55	54	
2	4	13	11	4	6	47	46	4	6	60	61	4	16	58	59	5	3	22	21	8	7	41	42	6	4	81	76	3	9	20	17	
2	6	19	19	6	0	21	22	4	8	14	17	4	18	74	74	5	4	58	59	1	9	35	36	6	5	16	13	3	10	18	18	
2	7	20	19	6	3	23	22	4	9	10	16	4	20	84	84	5	5	22	21	1	10	36	36	6	6	16	16	3	11	46	46	
2	8	43	41	6	4	27	26	4	1	22	21	4	22	84	84	5	6	38	37	1	11	46	45	6	7	17	18	3	12	46	46	
2	9	18	17	6	5	13	6	6	2	32	32	4	24	84	84	5	7	27	28	1	12	49	47	6	8	26	26	3	13	46	46	
4	0	34	33	6	3	12	13	6	3	12	13	4	26	84	84	5	8	22	22	1	13	49	47	6	9	35	36	3	14	46	46	
4	1	18	16	6	4	35	34	6	4	35	34	4	28	84	84	5	9	32	30	1	14	49	47	6	10	36	36	3	15	46	46	
4	2	21	22	6	5	22	21	6	5	22	21	4	30	84	84	5	10	32	30	1	15	49	47	6	11	36	35	3	16	46	46	
4	3	16	16	1	0	56	57	6	6	28	27	4	32	84	84	5	11	19	20	1	16	49	47	6	12	36	35	3	17	46	46	
4	4	47	45	1	2	54	54	6	7	21	23	4	34	84	84	5	12	11	11	1	17	46	45	6	13	36	35	3	18	46	46	
4	6	39	37	1	3	56	58	6	8	19	19	4	36	84	84	5	13	11	11	1	18	46	45	6	14	36	35	3	19	46	46	
H=-15				1	4	40	47	H=-11				4	2	103	107	H=-8				4	10	20	21	3	1	11	17	4	4	107	112	
				1	6	47	46					4	3	15	18	H=-8				4	12	49	47	4	5	9	9	7	2	41	43	
				1	8	54	59	1	0	31	34	4	4	48	100	0	0	58	55	3	0	22	21	4	6	75	76	7	4	71	71	
1	2	41	40	1	9	20	21	1	1	21	24	4	5	21	23	0	2	9	12	3	1	12	9	4	7	23	23	7	5	17	18	
1	3	13	12	1	10	31	29	1	2	53	55	4	6	27	30	0	4	149	153	3	2	34	37	4	8	26	26	7	7	12	13	
1	4	45	44	3	0	18	17	1	4	165	103	4	7	14	12	0	6	46	43	3	3	4	5	4	10	25	24	7	8	22	23	
1	5	25	25	3	2	41	41	1	5	48	48	4	10	54	05	0	10	84	83	3	4	28	31	6	0	29	28	9	0	37	38	
1	6	37	37	3	4	72	74	1	6	44	45	4	12	62	62	0	12	62	62	3	5	53	52	6	1	17	18	9	1	16	18	
1	9	29	26	3	5	42	42	1	7	54	55	6	1	26	26	2	4	53	54	3	6	15	14	6	2	55	52	9				

Table D. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	
H = -4				1	6	141	111	2	8	33	34	5	5	22	23	6	9	29	28	2	2	25	15	7	4	28	29	3	6	58	57	
0	0	56	72	1	7	22	19	2	9	49	51	5	6	26	27	8	0	58	60	2	3	102	91	7	5	12	13	3	7	17	15	
0	2	48	57	1	8	64	62	2	10	28	28	5	7	22	22	8	2	48	40	2	4	19	17	7	6	59	58	3	8	54	53	
0	4	81	85	1	9	40	40	2	11	23	22	5	8	52	53	8	3	21	18	2	5	71	73	9	1	15	16	3	9	15	15	
0	6	166	172	1	10	20	22	2	12	47	46	5	10	46	45	8	4	38	39	2	6	58	59	9	1	15	16	3	1	52	50	
0	10	19	18	1	12	30	31	4	0	169	164	7	0	16	14	8	5	19	18	2	7	23	22	9	2	33	32	5	2	39	42	
2	0	48	49	3	0	31	31	4	2	69	68	7	1	23	22	2	8	88	93	H = 4				8	2	315	299	5	4	41	41	
2	12	56	55	3	1	51	38	4	3	22	26	7	2	33	30	2	9	22	20	0	4	67	63	0	4	67	63	5	6	26	26	
2	0	48	49	3	2	51	89	4	4	49	48	7	3	12	11	4	10	31	32	0	6	84	83	0	8	104	103	5	7	31	33	
2	1	150	136	3	3	16	22	4	6	139	111	7	4	68	67	4	2	111	105	0	10	27	27	2	1	16	14	7	1	17	17	
2	2	30	39	3	4	152	153	4	7	24	24	7	6	51	49	4	5	15	16	2	9	22	20	2	4	38	41	7	6	18	19	
2	3	21	27	3	5	24	19	4	8	25	25	7	7	15	13	4	6	73	75	0	10	27	27	2	6	39	40	9	1	37	36	
2	4	103	99	3	6	40	42	4	10	14	12	9	0	39	40	4	8	106	108	2	1	16	14	2	4	38	41	9	2	37	36	
2	5	19	14	3	7	48	47	6	0	24	25	9	1	18	18	4	9	13	13	2	2	23	18	2	6	39	40	9	1	37	36	
2	6	75	79	3	8	9	6	6	1	17	22	9	2	50	52	6	2	41	41	2	7	41	39	2	8	46	44	9	2	37	36	
2	7	30	30	3	9	10	9	6	2	64	67	9	4	48	48	6	3	11	11	2	8	46	44	2	9	18	14	H = 6				
2	8	34	36	3	10	25	27	6	3	12	12	0	5	55	54	6	4	66	66	2	10	35	37	2	11	15	14	0	2	91	89	
2	9	21	22	3	12	62	61	6	4	55	54	0	6	103	103	6	5	25	26	2	11	15	14	4	1	15	15	0	4	133	141	
2	10	29	31	5	0	41	40	6	5	22	22	0	8	103	103	6	6	42	43	2	12	41	41	4	2	21	21	0	6	95	96	
2	11	26	26	5	1	22	23	6	7	25	23	0	10	16	14	6	7	22	22	4	3	30	31	4	3	65	59	0	8	49	50	
2	12	41	41	5	2	64	67	6	8	36	30	0	12	22	21	6	8	52	52	4	4	125	127	4	4	6	72	71	0	10	20	19
4	0	80	81	5	3	12	18	8	0	11	8	2	1	21	23	4	9	13	13	4	5	13	13	4	6	72	71	2	1	62	63	
4	1	94	94	5	4	97	97	8	1	34	34	2	3	59	88	4	10	22	24	4	6	70	71	4	7	30	32	2	2	129	122	
4	2	139	135	5	5	65	67	8	2	76	79	2	4	22	22	4	11	31	29	4	8	15	13	4	8	15	13	2	3	36	36	
4	4	111	112	5	6	69	70	8	3	17	15	2	5	37	37	5	12	27	19	4	9	24	21	4	9	24	21	2	4	41	39	
4	5	12	7	5	7	34	34	8	4	74	71	2	6	61	64	5	13	27	19	6	10	24	21	4	1	19	19	2	5	17	17	
4	6	48	48	5	8	41	42	8	5	29	27	2	7	34	32	5	14	44	44	6	11	21	21	6	2	68	69	2	7	71	72	
4	7	18	18	5	9	26	27	8	6	15	16	2	8	69	70	5	15	89	89	6	12	41	41	6	3	38	37	2	8	25	25	
4	8	70	71	5	10	39	39	8	7	46	47	2	9	43	43	5	16	88	90	6	13	46	46	6	4	38	37	2	10	45	44	
4	9	13	13	7	0	65	62	H = -1				2	10	42	44	5	17	74	74	6	14	46	46	6	5	14	11	4	1	9	9	
4	10	49	49	7	1	44	44	1	0	161	159	2	12	27	29	5	18	38	39	6	15	42	42	6	6	42	42	4	2	134	139	
4	11	21	21	7	2	65	63	1	1	21	33	2	13	27	29	5	19	48	48	6	16	43	43	6	7	48	47	4	4	55	54	
6	0	20	19	7	3	20	20	1	2	96	82	2	14	22	16	4	20	46	46	6	17	44	44	6	8	32	33	4	6	13	11	
6	1	63	63	7	4	41	42	1	3	161	156	2	15	20	20	4	21	47	47	6	18	45	45	6	9	24	26	4	8	44	43	
6	2	16	18	9	0	25	25	1	4	63	71	2	16	22	16	4	22	48	48	6	19	46	46	6	10	32	33	4	9	46	45	
6	3	43	47	9	1	41	42	1	5	59	58	2	17	23	23	4	23	49	49	6	20	47	47	6	11	32	33	4	10	48	47	
6	4	36	34	9	2	41	42	1	6	117	117	2	18	24	24	4	24	50	50	6	21	48	48	6	12	33	34	4	11	50	49	
6	5	30	32	9	3	25	26	1	7	46	47	2	19	25	25	4	25	51	51	6	22	49	49	6	13	34	35	4	12	51	50	
6	6	58	58	9	4	35	35	1	8	40	41	2	20	26	26	4	26	52	52	6	23	50	50	6	14	35	36	4	13	52	51	
6	7	27	26	H = -2				1	9	40	41	2	21	27	27	4	27	53	53	6	24	51	51	6	15	36	37	4	14	53	52	
6	8	25	25	0	0	147	142	1	10	52	52	2	22	28	28	4	28	54	54	6	25	52	52	6	16	37	38	4	15	54	53	
6	10	17	16	0	2	198	179	1	12	56	55	2	23	29	29	4	29	55	55	6	26	53	53	6	17	38	39	4	16	55	54	
6	0	43	42	0	3	148	147	3	0	194	183	2	24	30	30	4	30	56	56	6	27	54	54	6	18	39	40	4	17	56	55	
8	1	16	15	0	4	148	147	3	1	24	20	2	25	31	31	4	31	57	57	6	28	55	55	6	19	40	41	4	18	57	56	
8	2	37	37	0	5	77	77	3	2	131	131	2	26	32	32	4	32	58	58	6	29	56	56	6	20	41	42	4	19	58	57	
8	3	22	22	0	6	77	77	3	3	67	57	2	27	33	33	4	33	59	59	6	30	57	57	6	21	42	43	4	20	59	58	
8	4	47	48	0	10	63	62	3	4	34	34	2	28	34	34	4	34	60	60	6	31	58	58	6	22	43	44	4	21	60	59	
8	5	40	40	0	12	40	41	3	5	15	19	2	29	35	35	4	35	61	61	6	32	59	59	6	23	44	45	4	22	61	60	
H = -3				2	3	73	80	3	6	72	72	2	30	36	36	4	36	62	62	6	33	60	60	6	24	45	46	4	23	62	61	
1	0	131	133	2	1	191	196	3	7	35	34	2	31	37	37	4	37	63	63	6	34	61	61	6	25	46	47	4	24	63	62	
1	1	67	59	2	2	67	63	3	8	18	19	2	32	38	38	4	38	64	64	6	35	62	62	6	26	47	48	4	25	64	63	
1	2	50	45	2	3	51	45	3	9	83	84	2	33	39	39	4	39	65	65	6	36	63	63	6	27	48	49	4	26	65	64	
1	3	84	76	2	4	48	51	3	10	45	45	2	34	40	40	4	40	66	66	6	37	64	64	6	28	49	50	4	27	66	65	
1	4	46	35	2	5	65	67	3	11	79	80	2	35	41	41	4	41	67	67	6	38	65	65	6	29	50	51	4	28	67	66	
				2	6	84	86	3	12	105	105	2	36	42	42	4	42	68	68	6	39	66	66	6	30	51	52	4	29	68	67	
				2	7	15	18	3																								

Table D. (concluded)

[illegible]

Table E. Observed (FO) and Calculated (FC) Structure Factors for $[\text{Cu}_3(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC				
H=-14				H=-12																															
0	4	38	26	0	0	120	119	0	4	33	28	6	12	68	64	3	6	55	56	9	5	36	46	4	1	43	50	10	2	67	65				
1	1	40	39	0	2	47	53	0	6	58	53	7	1	84	85	3	7	47	47	9	7	36	37	4	2	47	54	10	6	57	52				
1	3	41	34	0	4	89	92	0	10	94	81	7	2	37	34	3	9	65	61	9	8	36	34	4	3	32	34	10	7	54	60				
1	4	38	34	0	6	74	69	1	2	46	49	7	3	54	56	3	10	87	80	9	10	64	59	4	5	48	51	10	9	36	28				
1	6	41	32	0	8	41	39	1	3	52	46	8	0	64	63	3	11	96	82	9	12	44	36	4	11	54	51	10	10	74	70				
2	0	64	66	0	10	46	35	1	4	61	61	8	1	56	57	3	13	77	67	10	0	50	53	4	12	37	37	11	0	87	81				
2	5	43	46	0	12	51	36	1	5	41	44	8	2	57	60	3	16	51	43	10	4	50	48	4	13	46	44	11	1	55	49				
2	7	72	64	0	14	44	34	1	10	69	62	8	4	80	83	4	0	78	81	10	6	105	105	4	10	75	66	11	2	63	64				
2	8	38	20	1	0	66	72	1	11	36	29	8	6	82	83	4	1	77	86	10	8	41	42	4	19	61	54	11	3	47	40				
3	4	41	37	1	1	90	96	1	16	42	34	9	0	80	93	4	5	43	46	11	5	55	61	5	0	41	39	11	4	50	44				
3	6	40	38	1	3	63	64	2	0	59	69	9	1	40	27	4	6	53	56	11	4	58	54	5	2	43	41	11	5	37	30				
3	7	38	33	1	7	70	58	2	2	54	66	9	5	64	59	4	7	54	51	5	5	62	62	5	5	62	62	11	6	40	37				
4	1	69	60	1	12	67	63	2	3	163	169	9	9	41	43	4	8	36	43	0	8	128	145	5	6	40	53	0	0	250	282				
4	3	41	39	2	2	42	43	2	4	49	53	10	2	46	54	4	9	64	67	0	2	85	91	5	7	30	24	0	2	66	76				
H=-13				2	3	33	30	2	6	111	105	10	4	36	35	4	10	43	45	0	4	105	199	5	10	98	103	0	2	66	76				
				2	4	61	67	2	7	33	22	4	14	40	36	0	6	160	169	5	13	52	49	0	4	85	86	0	4	85	86				
				2	5	76	72	2	9	78	73	4	15	36	35	0	8	222	203	5	17	68	59	0	6	80	85	0	6	80	85				
0	2	117	112	2	7	121	113	2	11	89	74	5	0	188	113	0	10	61	58	5	18	44	31	0	8	166	165	0	8	166	165				
0	6	48	29	2	8	89	82	2	13	43	33	0	0	213	236	5	1	93	99	0	12	131	117	6	0	116	118	0	10	136	12				
0	8	75	56	2	9	80	75	2	15	41	33	0	4	120	117	5	2	89	92	0	18	77	70	6	1	47	44	0	12	79	66				
0	10	46	26	2	10	58	44	3	0	82	91	0	6	54	56	5	3	37	21	0	20	52	40	6	4	36	42	0	14	98	90				
0	12	117	98	3	5	95	90	3	1	85	91	0	8	46	42	5	4	53	57	1	0	40	46	6	5	34	41	0	16	116	103				
1	0	35	27	3	6	70	65	3	2	57	60	0	10	73	71	5	5	39	47	1	2	59	69	6	6	118	119	1	0	75	43				
1	2	46	41	3	8	38	36	3	3	52	53	0	12	69	71	5	6	73	73	1	3	35	36	6	7	158	159	1	1	67	74				
1	4	55	54	3	9	57	48	3	6	65	67	0	14	97	86	5	7	39	52	1	4	153	155	6	8	70	56	1	2	159	179				
1	5	57	54	3	10	44	44	3	7	61	57	0	16	99	88	5	14	63	58	1	5	107	116	6	9	39	37	1	3	177	194				
1	8	70	67	3	11	49	45	3	10	57	44	0	18	90	76	5	17	46	32	1	6	35	35	6	10	33	31	1	4	62	67				
1	9	54	51	3	14	48	31	3	11	54	52	1	0	154	176	6	1	38	38	1	7	83	85	6	15	65	57	1	5	31	35				
1	11	74	59	4	0	34	38	3	12	35	40	1	1	32	20	6	2	40	32	1	9	91	94	7	0	76	85	1	6	10	26				
2	1	37	37	4	1	107	114	3	13	74	63	1	2	47	54	6	3	159	166	1	10	47	39	7	2	45	45	1	7	82	55				
2	3	70	67	4	2	54	57	3	14	46	43	1	3	88	87	6	5	45	44	1	11	134	125	7	3	178	186	1	8	87	82				
2	4	71	78	4	5	50	49	3	15	34	16	1	4	38	38	6	8	91	95	2	0	27	24	7	4	68	67	1	9	49	50				
2	5	86	81	4	8	47	38	3	17	50	44	1	6	33	22	6	10	60	55	2	1	27	22	7	5	47	51	1	10	47	41				
2	9	40	42	4	9	47	47	4	0	80	84	1	7	42	33	6	11	86	79	2	2	30	28	7	7	32	21	1	13	55	52				
2	11	58	42	4	14	45	35	4	2	48	49	1	8	42	40	6	15	10	28	2	3	135	141	7	11	60	54	1	14	72	62				
2	12	48	27	5	8	39	48	4	5	62	61	1	9	62	65	7	0	44	40	2	5	99	106	7	0	112	113	1	15	35	27				
2	13	45	22	5	2	52	57	4	8	61	49	1	11	44	39	7	2	38	31	2	7	53	38	8	1	79	82	1	19	44	38				
3	0	37	30	5	4	41	48	4	9	46	45	1	12	42	40	7	5	69	67	2	11	191	182	8	3	43	31	1	20	37	28				
3	1	83	81	5	9	70	65	4	13	53	49	1	13	52	51	7	8	33	16	2	14	45	30	8	4	80	80	2	0	89	103				
3	2	65	66	5	12	61	68	4	14	64	47	1	14	77	63	7	11	50	46	2	15	48	47	8	6	36	24	2	1	40	27				
3	9	43	38	5	13	72	64	4	16	43	37	1	15	62	50	7	14	54	37	3	0	66	76	8	7	85	79	2	3	47	35				
4	1	63	67	6	2	64	66	5	0	62	64	1	18	44	31	7	15	50	41	3	1	125	144	8	8	58	62	2	4	91	94				
4	5	59	52	6	3	71	79	5	4	81	78	2	1	39	43	8	0	48	54	3	2	101	110	8	10	54	42	2	5	55	59				
5	0	39	36	6	4	39	38	5	5	54	56	2	2	72	74	8	2	38	41	3	3	67	72	8	12	74	68	2	7	217	225				
5	2	42	35	6	8	74	70	5	6	48	56	2	4	47	47	8	4	98	91	3	5	96	102	8	13	47	40	2	8	47	49				
5	5	40	39	6	11	50	38	5	9	74	72	2	7	203	193	8	5	49	49	3	6	59	187	8	14	83	77	2	9	154	161				
5	6	56	57	7	1	51	51	5	10	86	83	2	8	36	27	8	6	63	61	3	8	48	53	9	0	103	107	2	10	113	108				
5	8	37	31	8	2	53	55	5	12	37	26	2	9	69	61	0	0	109	109	3	9	35	27	9	2	50	56	2	11	53	50				
5	9	36	27	8	6	39	35	5	13	38	35	2	12	38	37	8	9	37	33	3	10	51	49	9	7	54	57	2	12	60	54				
6	4	86	98					6	3	38	38	2	16	47	42	8	10	40	49	3	13	40	36	9	8	43	31	2	13	39	34				
6	5	46	36					6	4	56	59	3	2	62	76	0	11	41	34	3	14	63	76	9	9	43	51								

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
3	3	88	93	7	7	79	74	1	9	68	52	5	2	31	28	10	2	68	82	2	9	228	249	6	7	37	33	11	4	35	48	11	4	35	48
3	4	98	98	7	9	56	48	1	10	90	89	5	4	78	69	10	6	183	195	2	11	79	79	6	8	152	156	11	6	135	132	11	6	135	132
3	5	140	142	7	10	41	29	1	14	71	66	5	5	191	191	10	8	64	64	2	12	36	33	6	9	36	33	11	8	74	78	11	8	74	78
3	6	80	86	7	11	40	40	1	15	32	29	5	6	187	190	10	10	99	100	2	14	78	65	6	10	139	133	11	10	164	164	11	10	164	164
3	7	95	96	8	4	80	80	1	17	79	73	5	7	57	54	10	12	40	37	2	15	100	102	6	11	90	90	11	13	85	83	12	0	43	40
3	8	43	37	8	6	74	72	1	18	39	33	5	8	29	11	10	14	36	24	2	21	48	41	6	12	35	35	12	0	43	40	12	0	43	40
3	9	114	109	8	8	108	104	1	19	38	30	5	9	176	174	10	15	48	48	3	1	107	119	6	13	80	80	12	2	64	69	12	2	64	69
3	10	98	99	8	12	112	112	1	21	43	42	5	10	149	148	11	2	142	146	3	2	74	77	6	14	80	77	12	9	65	69	12	9	65	69
3	11	30	18	8	13	45	41	2	0	90	94	5	11	45	47	11	5	88	88	3	3	78	77	6	17	84	80	12	11	43	43	12	11	43	43
3	13	56	50	8	16	62	62	2	1	97	111	5	14	39	37	11	6	43	37	3	4	26	36	6	19	63	61	12	12	39	33	13	3	59	62
3	14	43	38	8	17	50	43	2	2	65	74	5	16	43	37	11	7	46	85	3	5	181	198	7	1	58	65	13	1	58	61	13	1	58	61
3	16	38	19	9	1	42	45	2	3	121	135	6	2	31	33	11	9	82	89	3	6	217	232	7	2	61	62	13	2	55	66	13	2	55	66
3	17	38	26	9	2	43	40	2	4	65	66	6	3	125	124	11	12	50	54	3	7	104	188	7	3	26	16	13	3	59	62	13	3	59	62
3	18	78	65	9	3	43	34	2	5	152	166	6	4	107	110	12	1	96	180	3	9	267	273	7	5	53	47	13	9	63	65	13	9	63	65
3	19	38	35	9	4	121	120	2	6	99	99	6	5	74	81	12	3	70	71	3	10	107	112	7	6	80	76	14	3	72	84	14	3	72	84
4	0	107	113	9	8	58	52	2	7	55	54	6	6	172	170	12	5	71	67	3	11	59	60	7	9	38	43								
4	1	133	142	9	10	62	65	2	9	67	67	6	7	152	150	12	6	61	59	3	12	36	38	7	10	53	52								
4	3	35	36	9	13	75	74	2	10	99	106	6	8	9	106	12	7	38	41	3	13	37	33	7	12	72	72								
4	4	119	131	10	0	72	74	2	11	203	202	6	10	141	139	13	2	62	65	3	14	55	52	7	13	111	110								
4	5	30	31	10	3	41	43	2	13	88	79	6	12	45	43	13	4	40	45	3	15	38	34	7	14	35	34								
4	8	41	41	10	6	82	83	2	17	64	55	6	13	88	83	13	5	61	68	3	16	33	31	7	15	39	40								
4	10	50	47	10	8	65	63	2	19	59	52	6	14	62	59					3	17	76	72	7	17	84	82								
4	14	42	42	10	9	37	46	2	20	46	34	6	15	85	83					3	18	41	40	7	19	38	22								
4	16	47	37	10	10	77	74	3	0	75	75	7	1	95	92					4	0	101	100	8	0	186	183								
4	17	88	81	11	0	60	58	3	1	147	156	7	3	110	113					4	1	167	167	8	2	98	95								
4	18	76	74	11	1	41	46	3	2	220	237	7	7	46	46					4	2	117	124	8	3	95	84								
5	1	74	74	11	2	47	48	3	3	258	273	7	8	79	77					4	3	125	126	8	4	188	189								
5	2	155	159	11	3	95	100	3	4	64	72	7	9	46	41					4	4	50	46	8	6	68	67								
5	4	46	41	11	4	65	65	3	5	68	57	7	10	31	24					4	5	144	139	8	7	52	41								
5	5	131	135	11	5	58	51	3	6	143	153	7	11	51	43					4	6	122	119	8	8	89	90								
5	6	38	41	11	6	88	85	3	7	66	73	7	12	38	37					4	7	30	23	8	9	50	41								
5	7	59	61	11	7	46	42	3	8	75	85	7	13	46	44					4	9	51	43	8	10	46	49								
5	8	79	77	11	9	38	28	3	10	86	89	7	15	42	39					4	10	53	48	8	12	53	54								
5	9	66	64	12	2	42	38	3	11	57	59	8	0	126	126					4	12	131	131	8	15	58	53								
5	11	30	16	12	3	68	62	3	13	156	146	8	1	32	22					4	13	58	56	8	16	60	50								
5	12	51	57	12	7	42	36	3	14	86	86	8	2	122	122					4	15	53	56	8	17	92	87								
5	13	60	60					3	19	48	40	8	3	110	106					4	28	49	38	9	0	99	101								
5	14	131	127					4	6	178	183	8	4	71	65					4	21	49	41	9	1	130	132								
5	15	79	69					4	1	110	115	8	8	94	92					5	1	107	109	9	2	48	47								
5	18	41	31					4	2	67	68	8	10	46	40					5	2	310	305	9	3	81	87								
6	2	83	79					4	3	91	87	8	12	100	94					5	3	137	142	9	6	206	198								
6	3	93	97					4	4	100	104	8	16	78	71					5	5	73	75	9	7	43	44								
6	4	36	36					4	5	61	57	8	17	62	62					5	6	27	16	9	9	50	49								
6	5	62	65					4	6	96	101	9	0	36	31					5	7	127	124	9	10	58	55								
6	6	153	152					4	7	45	41	9	1	36	39					5	8	53	53	9	11	38	36								
6	8	50	47					4	8	31	29	9	2	125	126					5	9	91	89	9	13	39	35								
6	9	32	29					4	10	56	53	9	4	36	27					5	10	98	92	9	14	41	44								
6	10	52	57					4	11	35	38	9	5	99	106					5	11	39	38	10	2	46	52								
6	11	181	178					4	12	40	44	9	6	45	41					5	12	58	61	10	4	108	106								
6	13	48	46					4	14	51	54	9	7	48	50					5	13	56	59	10	6	161	164								
6	15	58	50					4	15	38	44	9	8	62	53					5	14	115	119	10	7	52	45								
6	17	43	39					4	16	81	83	9	9	63	62					6	0	40	41	10	8	33	30								
7	1	64	65					4	17	62	61	9	11	45	54					6	2	46	48	10	10	76	73								
7	2	52	47					4	18	54	50	9	14	61	59					6	3	169	169	10	11	52	61								
7	3	130	129					4	21	39	29	9	15	37	42					6	5</														

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
2	14	40	36	5	19	42	39	9	12	75	79	1	8	63	74	4	10	80	81	8	2	94	98	13	6	65	74	3	5	175	161
2	15	50	61	6	0	40	35	9	13	40	45	1	9	25	18	4	12	36	26	8	3	41	30	14	1	78	81	3	6	154	148
2	17	77	75	6	1	146	139	9	14	96	97	1	10	115	123	4	13	72	68	8	4	144	141	14	3	87	101	3	7	30	22
2	18	36	41	6	2	92	85	10	3	137	135	1	11	36	35	4	14	41	36	8	5	55	48	14	4	62	70	3	8	47	47
2	19	52	54	6	3	244	237	10	4	137	141	1	12	48	45	4	15	66	68	8	6	78	75	14	5	87	97	3	9	150	145
2	20	44	42	6	4	52	58	10	5	32	20	1	13	68	70	4	16	66	63	8	7	51	54	14	6	58	60	3	10	198	191
2	21	38	32	6	5	67	65	10	7	53	49	1	14	105	115	4	17	43	37	8	8	242	235	3	10	197	191	3	11	49	56
2	22	40	36	6	6	122	116	10	8	57	59	1	15	49	44	4	20	111	114	8	9	89	87	3	11	49	56	3	13	87	92
3	1	272	203	6	7	145	144	10	9	37	47	1	16	106	104	4	21	38	42	8	11	44	39	3	14	67	66	3	15	129	131
3	2	238	244	6	8	135	126	10	10	78	76	1	18	39	39	5	0	147	134	8	12	147	144	0	0	115	138	3	16	67	71
3	3	59	49	6	9	130	128	10	14	91	93	1	21	72	64	5	1	165	166	8	15	50	44	0	2	197	241	3	18	56	57
3	4	29	21	6	10	66	63	11	0	113	114	2	0	110	119	5	2	192	181	8	18	58	49	0	4	212	252	3	19	102	103
3	5	45	33	6	11	44	38	11	1	37	27	2	1	78	74	5	3	94	89	8	19	49	41	0	6	209	246	4	0	184	171
3	6	57	61	6	12	63	70	11	2	98	97	2	2	90	91	5	4	86	85	9	0	31	27	0	8	377	420	4	1	86	85
3	7	113	119	6	15	41	40	11	5	51	48	2	3	127	117	5	5	94	83	9	1	84	81	0	10	107	108	4	2	309	292
3	8	51	54	6	16	58	56	11	6	65	70	2	4	69	69	5	6	88	87	9	2	70	71	0	12	180	191	4	3	129	124
3	9	79	81	6	17	62	58	11	7	60	64	2	5	31	23	5	8	39	33	9	3	56	55	0	14	67	64	4	6	72	68
3	10	151	155	6	18	46	42	11	9	61	61	2	6	40	49	5	9	60	59	9	4	118	115	0	16	70	68	4	7	190	178
3	11	147	148	6	19	35	25	11	10	105	106	2	7	167	191	5	10	142	137	9	6	87	85	0	18	43	42	4	8	190	178
3	12	44	47	6	21	81	73	11	11	40	24	2	9	279	301	5	11	117	114	9	7	48	47	0	20	151	151	4	9	12	44
3	13	150	150	7	0	86	84	11	14	74	83	2	10	85	92	5	12	134	139	9	9	76	78	0	22	94	92	4	12	47	44
3	14	138	144	7	1	141	136	12	0	80	96	2	11	70	76	5	13	115	113	9	12	113	109	1	0	116	132	4	13	38	43
3	15	70	73	7	2	37	29	12	3	79	82	2	12	47	48	5	14	103	103	9	13	63	61	1	1	161	183	4	14	72	71
3	17	35	38	7	3	137	133	12	4	37	38	2	13	76	77	5	15	100	98	9	14	58	60	1	2	83	99	4	15	47	44
3	18	54	57	7	4	92	85	12	13	44	39	2	14	30	29	5	16	72	70	9	15	66	66	1	3	172	193	4	16	96	98
3	22	37	22	7	5	131	126	13	1	38	34	2	17	58	54	5	18	69	66	10	1	98	99	1	4	223	251	4	18	50	49
4	0	94	90	7	7	66	60	13	2	90	97	2	18	41	43	5	19	42	45	10	2	80	83	1	5	156	171	4	19	83	82
4	1	111	106	7	8	32	31	13	3	46	46	2	22	53	53	6	0	73	71	10	5	111	111	1	6	115	124	4	20	48	49
4	2	125	127	7	9	68	64	13	5	73	72	3	0	139	135	6	1	159	148	10	6	49	51	1	8	40	21	5	0	170	152
4	3	45	46	7	10	84	81	13	7	49	53	3	1	94	83	6	2	94	90	10	7	63	59	1	10	74	75	5	1	236	222
4	4	114	117	7	11	48	47	13	10	45	41	3	2	76	82	6	3	173	162	10	8	166	166	1	11	74	78	5	2	184	174
4	5	51	48	7	12	52	47	14	1	40	33	3	3	38	38	6	4	179	171	10	10	60	62	1	12	167	179	5	3	74	69
4	6	27	4	7	13	122	114	14	2	48	53	3	4	105	107	6	5	232	223	10	12	58	57	1	13	83	93	5	4	212	201
4	7	91	88	7	14	36	37	14	3	88	92	3	5	327	323	6	6	123	116	10	14	48	48	1	14	42	40	5	5	280	262
4	8	50	46	8	0	196	194	14	4	46	33	3	6	198	199	6	7	224	212	11	0	51	57	1	17	105	113	5	6	250	247
4	9	95	92	8	1	117	112	14	7	102	111	3	7	140	136	6	8	119	117	11	1	138	139	1	22	42	46	5	7	123	112
4	11	57	53	8	2	67	68					3	8	94	90	6	9	70	63	11	2	125	124	1	23	50	49	5	9	36	39
4	14	90	86	8	3	174	171					3	9	32	37	6	10	84	81	11	5	37	32	2	0	85	90	5	10	75	73
4	15	51	56	8	4	147	147					3	10	114	117	6	11	164	166	11	6	109	112	2	1	369	372	5	11	115	108
4	17	59	57	8	8	77	78	8	0	478	547	3	11	167	163	6	13	162	160	11	9	50	56	2	2	110	112	5	12	146	146
4	19	88	83	8	9	118	103	0	2	269	309	3	12	78	85	6	15	34	38	11	10	39	36	2	3	196	199	5	13	40	42
4	20	73	74	8	10	107	101	0	4	417	473	3	13	62	57	6	17	74	72	11	11	43	38	2	5	204	218	5	14	41	39
5	1	51	52	8	12	46	44	0	6	36	37	3	14	96	101	7	0	147	140	11	12	59	60	2	6	44	37	5	15	78	84
5	2	71	68	8	15	86	81	0	8	114	126	3	15	38	26	7	1	280	201	11	13	72	74	2	8	231	242	5	16	105	106
5	3	53	49	8	16	89	96	0	10	77	77	3	17	126	128	7	2	42	40	11	14	41	36	2	9	74	74	5	22	49	48
5	6	253	247	9	0	52	54	0	12	57	56	3	18	71	78	7	3	35	33	11	15	61	64	2	10	107	116	6	0	84	77
5	7	110	109	9	2	152	146	0	14	40	45	3	19	32	24	7	5	231	215	11	16	59	49	2	11	192	207	6	3	129	119
5	9	81	78	9	3	47	50	0	16	113	106	3	21	44	46	7	6	30	25	12	1	62	68	2	13	223	231	6	4	217	211
5	11	59	60	9	4	33	41	1	0	232	279	4	1	62	62	7	7	50	48	12	3	68	64	2	14	46	44	6	5	176	165
5	12	76	77	9	5	90	86	1	1	257	313	4	2	192	185	7	8	31	26	12	4	74	78	2	15	78	85	6	7	240	234
5	13	85	86	9	6	106	109	1	2	131	148	4	3	181	98	7	9	48	43	12	7	55	59	2	16	50	53	6	8	138	133
5	14	33	33	9	7	40	39	1	3	151	173	4	4	33	34	7	10	44	45	12	8	66	61	2	20	38	48	6	9	310	305
5	15	41	37	9	8	40	40	1	4	34	14	4	5	59	61	7	12	35	35	12	9	85	86	3	0	201	179	6	10	60	59
5	16	56	52	9	9	36	39	1	5	73	86	4	6	162	156	7	17	51	50	12	10	45	37	3	1	489	484	6	11	77	71
5	17	89	87	9	10	76	73	1	6	97	112	4	8	85	83	8															

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
6	17	42	41	11	10	56	58	2	9	372	383	5	14	120	120	8	19	99	186	14	3	48	57	2	18	33	40	5	21	54	52				
7	1	148	137	11	11	72	82	2	10	59	61	5	15	61	56	8	20	69	71	14	4	62	66	2	19	36	35	5	22	56	63				
7	2	79	75	11	14	70	73	2	11	75	79	5	16	83	83	9	0	67	69	14	5	42	43	2	21	66	68	6	0	100	92				
7	3	50	46	11	16	44	44	2	12	49	55	5	18	60	62	9	1	101	102	14	7	42	31	3	1	286	253	6	2	54	51				
7	4	36	35	12	0	46	54	2	13	73	71	5	19	58	57	9	2	209	206	14	8	56	59	3	2	247	223	6	3	65	61				
7	5	151	149	12	1	154	162	2	15	98	107	6	0	27	13	9	3	134	133	14	9	43	50	3	3	545	508	6	4	26	22				
7	6	35	32	12	5	63	65	2	16	36	33	6	1	328	307	9	4	151	150	15	0	52	52	3	4	199	188	6	5	100	91				
7	7	85	81	12	8	80	92	2	17	96	107	6	3	209	188	9	6	145	142	15	1	39	23	3	5	79	84	6	6	99	98				
7	8	30	30	12	9	87	93	2	19	74	82	6	4	55	47	9	7	64	64	15	4	45	46	3	6	282	266	6	7	222	213				
7	9	146	140	13	1	38	44	3	0	143	123	6	5	177	173	9	9	38	33	3	7	269	248	6	8	147	147	6	8	147	147				
7	10	44	44	13	4	59	56	3	1	50	46	6	7	104	90	9	11	32	27	3	8	57	52	6	9	150	150	6	9	150	150				
7	11	67	62	13	5	127	136	3	2	400	370	6	8	186	180	9	12	72	79	3	9	236	233	6	10	162	162	6	10	162	162				
7	12	30	24	13	11	53	45	3	3	41	47	6	9	106	108	9	14	48	48	3	10	130	132	6	11	67	67	6	11	67	67				
7	13	35	35	13	12	77	75	3	4	171	157	6	10	37	37	9	15	53	49	3	11	28	23	6	12	144	147	6	12	144	147				
7	17	36	44	14	1	53	61	3	5	475	453	6	11	98	91	9	17	39	38	3	14	93	94	6	13	57	53	6	13	57	53				
7	18	35	34	14	5	50	53	3	6	259	252	6	12	175	178	18	0	104	100	3	15	159	157	6	15	67	67	6	15	67	67				
7	19	46	43	14	7	55	70	3	7	61	57	6	13	197	202	10	1	44	43	3	16	59	53	6	16	41	39	6	16	41	39				
8	0	131	126	14	8	75	81	3	8	79	73	6	14	31	42	10	2	57	59	3	18	63	68	6	17	123	129	6	17	123	129				
8	1	136	135	14	9	50	51	3	9	75	71	6	15	61	64	10	4	90	94	3	19	43	45	6	19	64	70	6	19	64	70				
8	2	41	33	15	0	53	61	3	10	91	90	6	16	37	33	10	5	53	51	3	21	37	22	7	0	43	41	7	0	43	41				
8	4	227	223	15	1	63	79	3	11	168	167	6	18	35	30	10	8	169	175	4	0	427	389	7	3	138	131	7	3	138	131				
8	5	75	69					3	13	53	43	6	21	46	40	18	9	46	50	4	1	134	122	7	4	29	25	7	4	29	25				
8	6	164	162					3	14	75	77	7	0	51	44	10	10	84	67	4	2	84	67	7	5	175	166	7	5	175	166				
8	9	29	28					3	16	31	32	7	1	85	88	18	11	60	58	4	4	38	23	7	6	128	121	7	6	128	121				
8	11	56	50					3	18	43	41	7	2	67	59	10	12	63	69	4	5	101	104	7	7	145	136	7	7	145	136				
8	12	174	166					3	19	86	88	7	3	46	49	10	13	77	85	4	6	28	31	7	8	27	28	7	8	27	28				
8	13	32	36					3	21	39	35	7	4	86	82	10	15	60	56	4	7	92	90	7	9	113	113	7	9	113	113				
8	15	34	40					3	22	65	71	7	5	147	139	10	16	56	60	4	8	71	65	7	10	55	60	7	10	55	60				
8	16	67	71					3	23	45	48	7	6	67	65	11	0	62	63	4	9	105	107	7	11	104	99	7	11	104	99				
8	19	52	55					4	4	292	274	7	7	57	52	11	1	125	133	4	10	110	114	7	13	43	43	7	13	43	43				
9	0	195	191					4	1	332	315	7	8	80	81	11	2	82	77	4	11	90	97	7	14	75	74	7	14	75	74				
9	1	79	72					4	2	291	264	7	9	114	109	11	3	124	128	4	12	114	113	7	15	110	111	7	15	110	111				
9	2	125	115					4	3	51	50	7	11	64	60	11	4	130	126	4	13	44	42	7	17	78	77	7	17	78	77				
9	3	34	34					4	4	37	31	7	13	54	49	11	5	36	40	4	15	29	25	8	0	373	368	8	0	373	368				
9	5	166	165					4	5	46	43	7	15	122	118	11	6	120	128	4	17	73	75	8	1	239	227	8	1	239	227				
9	7	99	99					4	8	252	245	7	16	66	64	11	7	42	41	4	18	74	75	8	3	169	159	8	3	169	159				
9	9	41	32					4	9	28	29	7	17	95	98	11	9	95	95	4	19	74	72	8	4	82	79	8	4	82	79				
9	10	41	45					4	10	83	84	7	20	40	37	11	10	124	128	4	20	39	55	8	5	165	168	8	5	165	168				
9	11	106	111					4	12	28	27	7	21	43	43	11	14	43	43	4	22	73	71	8	6	29	27	8	6	29	27				
9	16	145	146					4	13	101	98	8	0	149	149	12	0	64	67	5	0	96	87	8	7	62	61	8	7	62	61				
10	2	87	84					4	14	127	124	8	1	189	184	12	1	122	126	5	1	45	35	8	9	54	53	8	9	54	53				
10	4	84	87					4	15	76	77	8	2	85	77	12	4	72	78	5	2	214	198	8	10	44	48	8	10	44	48				
10	6	76	83					4	19	38	37	8	3	38	25	12	5	50	49	5	3	207	188	8	11	84	81	8	11	84	81				
10	7	37	32					4	22	56	58	8	4	156	153	12	6	41	32	5	4	254	236	8	12	204	210	8	12	204	210				
10	8	109	116					5	0	106	96	8	5	133	130	12	7	81	86	5	5	68	65	8	13	73	70	8	13	73	70				
10	10	50	50					5	1	245	220	8	6	202	201	12	10	37	35	5	6	143	140	8	15	71	75	8	15	71	75				
10	11	81	84					5	2	122	113	8	8	212	210	12	12	38	51	5	7	41	45	8	16	114	121	8	16	114	121				
10	12	106	106					5	3	192	184	8	9	54	46	12	13	36	27	5	8	164	161	8	17	38	43	8	17	38	43				
10	15	61	68					5	4	211	204	8	10	54	54	13	0	55	62	5	9	88	87	8	18	40	44	8	18	40	44				
11	0	41	40					5	5	131	126	8	11	63	57	13	1	54	60	5	10	135	142	8	19	46	51	8	19	46	51				
11	2	146	149					5	6	92	92	8	12	48	54	13	3	87	101	5	11	90	91	8	20	51	55	8	20	51	55				
11	4	54	51					5	7	162	155	8	13	39	41	13	4	73	82	5	13	100	90	9	0	35	34	9	0	35	34				
11	5	204	203					5	8	106	95	8	15	69	70	13	9	62	68	5	16	64	66	9	1	59	61	9	1	59	61				
11	6	50	40					5	9	94	91	8	16	84	85	13	10	37	45	5	18	57	58	9	2	51	42	9	2	51	42				
11	7	43	47					5	10	85	82	8	17	49	49	14	0	50	55	5	19	87	89	9	3	40	48	9	3	40	48				
11	8	45	44					5	12	90	95	8	18	55	53	14	2	41	44	5	20	51	41	9	4	251	256	9	4	251	256				

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
9	5	48	53	15	4	74	84	3	10	225	222	6	11	198	199	10	16	46	47	1	16	33	37	5	5	30	24	9	4	94	93				
9	6	98	101					3	11	154	155	6	12	52	55	11	2	120	123	1	17	63	66	5	5	26	24	9	5	117	119				
9	7	52	56					3	13	83	84	6	13	140	139	11	3	130	134	1	18	71	72	5	6	259	262	9	7	159	156				
9	8	123	124					3	14	65	68	6	14	69	73	11	4	147	148	1	19	68	68	5	7	267	261	9	9	38	44				
9	9	39	34					3	15	110	114	6	15	65	63	11	4	96	101	2	1	119	110	5	8	217	243	9	11	65	68				
9	10	47	47					3	17	77	74	6	16	67	76	11	9	89	94	2	3	213	228	5	10	185	182	9	12	151	158				
9	12	51	52					3	18	45	46	6	17	91	98	11	10	75	79	2	4	115	135	5	11	188	185	9	14	108	108				
9	13	42	44					3	19	85	89	6	21	50	48	11	11	50	59	2	5	181	202	5	14	58	51	9	18	36	43				
9	14	60	62					3	20	37	28	7	1	95	90	11	13	41	55	2	6	64	65	5	15	79	75	18	1	72	74				
9	16	72	75					3	23	47	55	7	2	37	29	11	15	97	107	2	7	60	77	5	16	96	101	18	2	59	54				
10	0	145	143					4	0	367	314	7	3	313	299	11	16	44	39	2	8	125	128	6	1	260	235	10	3	35	34				
10	1	75	77					4	1	153	134	7	4	168	164	12	1	79	47	2	9	26	25	6	2	149	133	10	5	78	78				
10	2	85	82					4	2	33	30	7	5	157	153	12	2	38	47	2	10	137	144	6	3	263	248	10	6	125	138				
10	3	114	116					4	3	145	138	7	6	37	34	12	4	64	74	2	11	328	341	6	4	29	4	10	7	66	65				
10	4	34	32					4	4	380	355	7	8	61	81	12	5	127	135	2	12	112	117	6	5	294	281	10	8	66	78				
10	5	52	52					4	5	143	145	7	9	70	71	12	11	45	47	2	13	83	88	6	6	192	184	10	10	120	123				
10	6	100	94					4	6	117	130	7	13	32	33	12	12	54	65	2	14	83	85	6	7	284	264	10	11	51	57				
10	7	74	79					4	7	45	43	7	15	79	77	12	14	55	63	2	15	120	118	6	9	186	173	10	12	36	48				
10	8	122	126					4	8	84	76	7	16	34	26	13	3	110	121	2	16	92	96	6	10	80	79	10	14	42	46				
10	9	47	42					4	9	50	55	7	19	74	72	13	4	47	45	2	17	75	78	6	11	113	108	10	15	63	65				
10	10	39	29					4	10	98	92	8	0	64	68	13	5	42	38	2	18	47	49	6	12	100	100	10	16	64	66				
10	12	114	117					4	11	206	206	8	1	259	248	13	7	35	31	2	20	41	36	6	13	56	54	11	1	129	131				
10	13	33	31					4	12	99	98	8	2	60	57	13	8	38	47	2	21	47	48	6	14	39	34	11	2	88	95				
10	14	90	92					4	13	34	37	8	3	67	56	13	11	44	47	3	1	91	90	6	15	57	55	11	3	73	72				
11	0	48	47					4	14	73	68	8	4	248	241	14	0	184	115	3	2	359	331	6	17	34	39	11	4	75	71				
11	2	156	155					4	15	104	101	8	5	84	86	14	1	92	97	3	3	396	392	6	18	46	43	11	7	159	171				
11	4	59	65					4	18	97	100	8	6	131	128	14	3	84	93	3	4	147	148	6	21	49	53	11	10	87	92				
11	5	93	98					4	20	49	51	8	7	47	49	14	5	93	106	3	6	136	141	7	2	60	65	11	11	76	80				
11	6	142	147					4	21	72	65	8	8	146	147	14	6	51	57	3	7	141	146	7	3	261	248	11	14	141	148				
11	7	69	73					4	22	63	64	8	9	28	35	15	2	61	65	3	8	28	22	7	4	26	27	11	16	42	31				
11	10	61	65					5	1	78	71	8	10	39	36	15	4	68	64	3	9	29	26	7	5	149	141	12	1	51	51				
11	11	49	54					5	2	158	139	8	12	62	62					3	10	105	110	7	6	88	74	12	2	41	49				
11	13	76	76					5	3	156	140	8	13	37	42					3	11	166	178	7	7	129	121	12	3	131	135				
11	14	54	62					5	4	216	206	8	14	87	97					3	12	96	98	7	8	46	44	12	4	73	75				
11	15	37	40					5	5	83	80	8	16	103	111					3	13	121	124	7	9	39	30	12	5	105	105				
12	0	80	86					5	6	130	123	8	17	62	62					3	14	134	140	7	11	73	67	12	7	35	39				
12	1	130	139					5	7	161	158	8	18	38	48					3	15	186	196	7	14	36	37	12	8	51	56				
12	8	39	51					5	8	223	221	8	19	38	38					3	17	31	35	7	18	36	30	12	10	57	68				
12	11	61	67					5	9	183	173	9	1	59	52					4	1	295	275	7	19	84	78	12	11	99	104				
13	0	41	49					5	10	40	71	9	3	105	109					4	2	146	174	8	1	51	51	13	3	39	50				
13	1	56	56					5	11	179	179	9	4	70	75					4	3	180	168	8	2	42	34	13	7	106	116				
13	2	35	34					5	13	70	75	9	5	61	57					4	4	284	284	8	3	114	108	13	8	99	98				
13	4	49	55					5	14	161	171	9	6	124	124					4	5	55	68	8	4	191	190	13	11	48	52				
13	5	91	95					5	15	100	105	9	8	220	224					4	6	39	40	8	5	145	139	14	1	103	118				
13	6	47	54					5	16	33	27	9	9	72	71					4	7	112	139	8	6	52	51	14	4	53	52				
13	7	91	98					5	21	41	40	9	10	156	163					4	8	59	46	8	7	222	215	14	5	36	34				
13	8	36	40					6	0	185	169	9	11	59	61					4	9	61	66	8	8	58	63	14	6	41	45				
13	11	56	60					6	1	232	211	9	15	59	64					4	10	106	113	8	9	58	63	14	7	59	72				
14	0	61	58					6	2	108	108	10	1	145	150					4	11	106	113	8	10	58	63	14	8	38	39				
14	1	44	43					6	3	271	264	10	2	40	45					4	12	109	111	8	11	58	63	14	9	46	53				
14	3	82	90					6	4	31	7	10	3	61	65					4	13	161	161	8	12	61	61	14	10	46	53				
14	5	38	35					6	5	47	44	10	4	56	53					4	14	166	166	8	13	59	65	14	11	46	53				
14	7	69	69					6	6	190	191	10	5	38	46					4	15	174	174	8	14	51	51	14	12	46	53				
14	8	82	88					6	9	192	194	10	6	106	108					4	16	166	166												

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
0	8	471	439	4	4	195	183	7	13	44	38	12	5	54	55	2	11	221	206	6	9	257	252	10	16	60	52	2	5	35	24
0	10	111	104	4	5	171	155	7	14	32	30	12	6	76	81	2	13	197	188	6	10	252	246	11	1	31	13	2	6	105	98
0	12	170	169	4	6	129	124	7	15	86	83	12	8	38	46	2	15	61	55	6	12	66	62	11	2	222	228	2	7	54	56
0	14	129	133	4	7	54	55	7	16	83	82	12	13	41	41	2	17	42	44	6	13	61	61	11	3	38	32	2	8	37	36
0	16	100	104	4	10	122	113	7	17	112	108	13	1	49	46	2	18	43	42	6	14	72	73	11	5	91	96	2	9	416	402
0	18	100	111	4	11	34	34	8	1	77	68	13	3	66	74	2	19	45	54	6	15	113	112	11	6	72	68	2	10	111	103
0	20	43	44	4	12	76	71	8	2	91	89	13	4	60	59	2	20	65	63	6	17	42	49	11	7	88	96	2	11	93	91
1	1	39	35	4	15	74	65	8	3	167	167	13	6	81	86	3	1	367	334	6	19	58	52	11	8	45	41	2	14	178	174
1	2	269	265	4	16	34	35	8	4	329	327	13	7	42	51	3	2	334	302	7	2	108	96	11	11	36	34	2	15	96	91
1	3	130	129	4	17	75	74	8	5	34	24	13	10	54	58	3	3	370	339	7	3	30	28	11	12	76	69	2	16	49	41
1	4	118	90	4	19	91	89	8	6	70	61	13	11	60	59	3	4	40	36	7	5	46	50	11	15	51	58	2	17	88	88
1	5	171	161	4	22	64	63	8	7	56	56	14	1	46	58	3	5	64	61	7	6	56	57	12	1	61	66	2	20	68	67
1	6	134	124	5	1	126	112	8	8	124	121	14	3	46	51	3	6	38	31	7	7	181	176	12	2	41	44	3	1	66	63
1	7	60	53	5	2	247	242	8	9	60	54	14	5	88	97	3	7	26	10	7	8	43	44	12	3	39	46	3	2	187	183
1	8	41	35	5	3	199	187	8	10	110	109	14	7	42	49	3	8	38	28	7	9	114	110	12	7	84	92	3	3	336	320
1	9	170	159	5	4	96	80	8	11	54	52	14	9	46	48	3	9	32	34	7	10	50	47	12	9	62	65	3	4	42	39
1	10	34	33	5	5	30	29	8	12	75	78	15	1	43	36	3	10	141	133	7	11	74	81	13	1	43	42	3	5	166	153
1	11	157	147	5	6	129	115	8	14	35	32					3	11	186	180	7	12	79	82	13	2	102	109	3	6	322	303
1	12	205	196	5	7	41	41	8	15	50	51	H= 3				3	14	82	85	7	13	189	188	13	3	38	29	3	7	283	263
1	13	139	131	5	8	122	113	8	17	66	69					3	15	44	46	7	14	71	75	13	5	58	75	3	9	29	27
1	14	120	113	5	9	160	152	8	19	60	63					3	16	39	39	7	16	41	35	13	7	64	73	3	10	74	67
1	15	120	118	5	10	84	78	9	1	66	67					3	17	108	114	7	17	37	21	13	10	52	58	3	11	181	166
1	16	102	101	5	11	104	99	9	3	183	157					3	21	44	45	8	1	54	43	14	1	53	59	3	13	90	87
1	18	64	60	5	12	29	18	9	6	110	109					4	2	160	141	8	2	183	175	14	4	60	55	3	14	90	89
2	1	291	270	5	13	29	28	9	8	132	131					4	3	332	320	8	3	210	205	14	5	88	100	3	16	35	39
2	2	203	185	5	14	199	199	9	10	34	38					4	4	29	19	8	4	34	31	14	7	37	27	3	17	84	82
2	3	310	274	5	15	101	99	9	13	57	58					4	5	134	129	8	5	73	64					3	19	58	56
2	5	200	170	5	17	58	44	9	14	54	58					4	6	118	109	8	6	91	87					3	21	43	43
2	6	159	147	5	19	38	39	9	16	45	41					4	7	128	114	8	7	70	72					4	1	158	144
2	7	148	132	6	1	221	208	9	18	84	87					4	8	181	171	8	8	156	156					4	2	217	199
2	8	40	34	6	2	31	25	10	2	45	54					4	9	89	84	8	9	79	79					4	4	101	91
2	9	356	332	6	3	80	77	10	3	31	39					4	11	63	54	8	10	45	42					4	5	49	52
2	10	39	40	6	4	52	43	10	4	84	86					4	12	49	48	8	11	70	71					4	6	172	165
2	11	120	113	6	5	366	338	10	6	38	47					4	13	36	35	8	12	141	145					4	7	385	289
2	15	154	144	6	6	117	117	10	7	70	78					4	14	95	94	8	14	51	50					4	8	95	98
2	16	70	65	6	9	97	96	10	8	79	78					4	15	47	50	8	16	101	107					4	9	92	88
2	19	51	46	6	10	143	134	10	9	66	71					4	17	84	81	8	17	84	81					4	10	188	181
2	21	68	61	6	11	165	162	10	10	164	167					4	20	52	54	9	2	182	184					4	11	95	93
2	22	50	55	6	12	51	43	10	11	93	92					4	21	69	71	9	3	50	49					4	13	42	38
3	1	243	218	6	13	66	70	10	12	50	45					5	1	65	59	9	5	47	52					4	14	69	68
3	2	257	226	6	14	106	99	10	15	34	10					5	2	56	48	9	6	134	133					4	15	70	76
3	3	173	158	6	15	71	66	11	1	75	74					5	3	131	114	9	7	94	96					4	16	48	43
3	4	77	67	6	16	73	74	11	2	60	58					5	5	135	126	9	9	38	43					4	20	91	88
3	5	270	237	6	17	50	55	11	3	126	133					5	6	319	311	9	10	50	50					5	1	55	49
3	6	189	168	6	20	50	47	11	4	47	56					5	7	38	32	9	11	40	35					5	2	249	234
3	7	289	265	7	1	48	47	11	6	95	102					5	9	34	24	9	14	51	56					5	3	157	148
3	8	159	150	7	2	27	15	11	7	60	60					5	13	74	72	9	16	96	100					5	4	108	99
3	9	121	107	7	3	58	68	11	8	51	55					5	15	78	81	10	2	69	68					5	5	109	97
3	10	101	93	7	4	47	48	11	10	83	87					5	18	120	125	10	3	98	94					5	6	40	35
3	11	127	119	7	5	59	49	11	11	75	83					5	19	100	97	10	4	32	26					5	7	144	138
3	13	105	97	7	6	30	36	11	12	64	75					6	1	188	176	10	5	38	43					5	9	120	115
3	15	133	127	7	7	199	187	11	15	50	60					6	2	55	51	10	6	164	170					5	10	235	227
3	18	123	118	7	8	30	28	12	1	90	91					6	3	129	120	10	7	38	4					5	11	89	88
3	19	95	97	7	9	62	62	12	2	42	38					6	4	47	39	10	9	72	76					5	12	49	49
4	1	32	28	7	11	137	133	12	3	170	176					6	5	87	78	10	14	109	116					5	13	37	25
4	2	210	187	7	12	57	57	12	4	53	57					6	8	76	70	10	15	48	42					5	14	96	96

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
5	16	47	48	10	12	69	74	2	12	161	155	6	4	127	121	13	1	56	52	3	11	172	160	7	7	43	40	13	2	60	64
5	17	188	112	10	14	53	52	2	13	272	264	6	5	111	106	13	3	60	63	3	12	53	48	7	8	74	68	13	4	58	67
5	18	42	32	10	15	48	47	2	15	42	45	6	6	33	29	13	7	74	82	3	14	68	63	7	9	41	37	13	5	88	72
6	1	146	140	11	2	95	97	2	16	51	52	6	9	233	231	14	1	68	77	3	15	31	23	7	11	34	38	13	6	83	83
6	2	140	131	11	3	60	65	2	18	38	42	6	10	85	90					3	16	27	26	7	12	45	44	13	7	33	39
6	3	45	38	11	4	72	72	2	19	58	51	6	11	85	85					3	17	41	34	7	13	82	81	14	1	58	54
6	4	48	46	11	6	165	169	3	1	49	42					H= 6				3	18	34	32	7	17	116	118				
6	5	171	162	11	8	39	46	3	2	192	175	6	12	95	99	0	2	347	393	4	1	68	58	8	1	165	156				
6	6	82	81	11	9	75	79	3	3	145	137	6	18	92	90	0	4	118	133	4	2	285	265	8	2	37	24				
6	7	46	44	11	11	69	78	3	4	150	137	7	1	231	226	0	6	186	204	4	3	81	77	8	3	89	87	0	2	64	71
6	8	174	169	12	3	138	145	3	5	198	189	7	2	96	94	0	8	137	137	4	4	107	102	8	4	165	160	0	4	351	374
6	9	31	23	12	4	43	45	3	6	116	109	7	4	70	70	0	10	146	155	4	5	110	102	8	5	81	78	0	6	293	317
6	10	59	62	12	5	50	53	3	7	83	75	7	5	67	66	0	12	76	78	4	6	160	154	8	6	87	91	0	8	182	195
6	11	35	34	12	10	37	36	3	8	76	73	7	9	102	106	0	14	125	131	4	7	106	98	8	7	71	63	0	10	25	27
6	13	226	221	12	11	45	47	3	9	161	156	7	10	37	34	0	16	112	112	4	8	87	81	8	8	66	73	0	12	48	59
6	14	106	109	13	3	97	103	3	10	182	180	7	11	53	53	0	20	61	58	4	9	38	30	8	11	59	55	0	14	45	51
6	18	49	49	13	6	57	70	3	11	88	87	7	13	38	40	1	1	93	102	4	10	43	43	8	12	34	38	1	1	164	170
7	2	78	76	14	1	50	59	3	13	93	84	8	1	95	94	1	2	180	185	4	11	123	120	8	13	34	35	1	2	31	24
7	3	144	136	14	2	66	72	3	14	34	30	8	2	94	90	1	3	69	74	4	13	25	26	8	16	33	29	1	3	107	109
7	4	130	125	14	5	74	82	3	15	65	65	8	3	146	140	1	4	191	196	4	14	40	39	9	1	73	72	1	4	35	34
7	5	186	182					3	16	38	33	8	4	149	152	1	5	63	61	4	15	150	148	9	2	34	35	1	5	206	213
7	7	85	77					3	17	97	99	8	5	74	69	1	6	101	97	4	19	41	45	9	3	78	80	1	6	78	76
7	8	30	30					4	1	146	145	8	7	120	120	1	7	42	53	5	1	47	47	9	4	83	75	1	7	106	104
7	9	101	94					4	2	347	335	8	8	36	45	1	8	97	101	5	2	28	24	9	6	49	40	1	8	213	211
7	10	51	49					4	3	211	199	8	9	50	45	1	9	162	167	5	3	127	120	9	8	143	146	1	9	22	22
7	17	124	129					4	4	116	102	8	10	106	111	1	10	113	107	5	4	125	115	9	9	44	37	1	10	137	135
8	1	177	167					4	5	161	158	8	14	107	114	1	11	49	44	5	5	150	148	9	10	81	75	1	11	48	44
8	2	127	123					4	6	163	154	8	15	52	57	1	12	64	60	5	6	48	40	9	12	62	61	1	12	101	98
8	3	221	215					4	7	31	34	8	16	48	49	1	15	64	64	5	7	124	118	9	14	44	35	1	13	58	61
8	4	122	115					4	8	30	25	9	1	67	69	1	16	75	74	5	8	41	38	10	1	70	75	1	15	40	43
8	5	33	14					4	9	45	42	9	2	35	27	1	18	36	37	5	9	75	69	10	2	54	45	1	17	46	49
8	6	111	110					4	11	188	182	9	3	64	64	2	1	88	79	5	10	187	178	10	3	53	63	2	1	308	301
8	7	38	40					4	13	56	51	9	4	123	121	2	2	182	177	5	11	54	48	10	4	27	18	2	2	107	104
8	8	108	115					4	14	75	77	9	5	52	51	2	3	28	24	5	12	52	54	10	7	67	62	2	3	91	91
8	9	55	63					4	15	63	68	9	7	85	86	2	5	119	114	5	14	50	48	10	8	60	58	2	4	86	86
8	10	123	126					4	16	69	72	9	8	58	64	2	6	85	81	5	15	39	38	10	9	51	46	2	5	46	46
8	11	43	47					4	17	56	56	9	10	95	100	2	7	71	75	5	16	57	55	10	10	67	72	2	6	29	29
8	12	109	113					4	18	39	37	9	11	44	42	2	8	201	189	5	18	78	73	10	12	120	128	2	7	21	3
8	16	52	57					4	19	90	93	9	16	45	49	2	9	196	182	8	1	311	290	10	13	48	58	2	8	40	38
9	1	42	50					4	20	68	69	10	2	122	125	2	10	44	36	6	2	29	13	11	2	46	42	2	11	126	125
9	2	38	34					5	2	180	169	10	3	45	43	2	11	112	102	6	3	57	59	11	3	33	34	2	12	79	78
9	3	42	32					5	3	308	292	10	8	139	143	2	12	80	78	6	4	84	72	11	5	112	114	2	13	152	145
9	4	63	57					5	4	29	21	10	11	53	64	2	13	139	128	6	5	97	86	11	6	89	93	2	14	35	33
9	5	41	42					5	6	295	285	10	14	142	150	2	14	44	40	6	8	91	87	11	7	62	64	2	15	29	12
9	6	218	222					5	7	224	215	11	2	39	44	2	16	66	65	6	10	46	41	11	8	67	72	2	16	45	46
9	8	42	41					5	8	85	79	11	3	108	114	2	17	121	113	6	12	69	55	11	9	57	64	2	17	34	42
9	9	61	65					5	9	30	33	11	4	97	98	3	1	54	44	6	13	125	123	11	10	36	40	2	18	74	78
9	11	80	85					5	11	89	87	11	5	90	103	3	2	154	151	6	14	125	123	11	11	49	45	3	1	65	54
9	12	96	102					5	12	65	63	11	7	109	112	3	3	183	91	6	15	40	35	11	12	75	70	3	2	77	75
9	14	56	52					5	14	69	71	11	10	90	97	3	4	32	27	6	16	97	95	12	1	149	148	3	3	95	92
10	1	91	91					5	15	35	20	12	1	57	59	3	5	189	174	7	1	40	43	12	2	31	35	3	4	76	76
10	4	92	98					5	16	56	63	12	3	104	103	3	6	133	127	7	2	84	75	12	3	85	91	3	5	131	127
10	5	57	61					5	18	51	55	12	5	46	44	3	7	169	150	7	3	88	79	12	4	52	51	3	6	62	59
10	6	49	57					6	1	121	113	12	7	112	118	3	8	123	120	7	4	32	21	12	5	53	65	3	7	119	114
10	7	37	31					6	2	34	34	12	10	54	56	3	9	86	81	7	5	260	250	12	6	62	53	3	9	29	26
10	10	162	169					6	3	141	134	12	11	73	79	3	10	40	40	7	6	46	40	12	9	60	55	3	10	104	97

Table E. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
3	11	82	77	8	1	107	93	1	13	70	71	5	15	38	41																								
3	12	52	51	8	2	176	167	1	14	42	45	5	16	47	49																								
3	13	81	84	8	3	27	31	1	15	62	59	6	1	155	146																								
3	14	47	51	8	4	71	65	1	16	90	94	6	2	117	111																								
3	15	79	78	8	5	172	169	1	17	64	66	6	4	60	66																								
3	16	30	30	8	7	70	66	2	1	32	24	6	5	94	86																								
3	18	40	37	8	8	74	68	2	2	40	41	6	6	34	32																								
4	1	200	183	8	11	40	41	2	3	33	25	6	7	28	19																								
4	2	189	181	8	12	93	95	2	4	59	52	6	8	106	102																								
4	3	154	145	8	13	68	63	2	5	208	205	6	9	126	121																								
4	6	56	51	8	15	48	51	2	6	53	53	6	11	52	54																								
4	7	71	66	9	2	64	62	2	7	70	71	6	12	46	44																								
4	8	46	39	9	3	42	40	2	9	117	112	6	13	87	84																								
4	10	127	124	9	4	90	96	2	10	56	59	6	15	32	33																								
4	11	117	111	9	5	91	85	2	11	78	77	7	1	139	136																								
4	12	27	25	9	6	72	70	2	14	47	47	7	3	25	25																								
4	13	39	40	9	7	45	43	2	15	57	63	7	4	34	27																								
4	15	79	80	9	10	37	34	2	16	105	105	7	5	112	107																								
4	16	53	54	9	12	74	78	2	17	52	52	7	6	60	69																								
4	17	34	40	9	13	33	28	3	1	97	89	7	7	101	98																								
5	1	22	16	10	1	26	24	3	2	153	149	7	10	74	68																								
5	2	161	151	10	2	127	123	3	3	90	81	7	11	64	63																								
5	3	24	14	10	3	50	48	3	6	68	60	7	12	31	10																								
5	4	114	112	10	5	103	103	3	7	49	47	7	13	116	113																								
5	5	58	55	10	6	33	40	3	8	69	68	8	1	168	162																								
5	6	113	108	10	8	93	94	3	9	144	141	8	2	65	62																								
5	7	34	28	11	1	37	37	3	10	36	37	8	3	128	128																								
5	8	108	102	11	2	55	62	3	11	31	27	8	4	112	120																								
5	9	61	62	11	4	60	57	3	12	30	27	8	5	103	94																								
5	10	24	19	11	8	50	53	3	14	44	44	8	6	124	117																								
5	11	62	69	11	9	56	59	4	1	120	107	8	7	41	39																								
5	12	31	30	11	10	30	18	4	3	122	115	8	8	106	106																								
5	14	71	71	12	1	82	83	4	4	99	95	8	10	48	41																								
5	15	63	63	12	2	75	76	4	5	107	96	8	12	48	42																								
5	16	37	40	12	5	75	75	4	6	118	110	9	1	27	35																								
6	1	56	52	13	2	38	31	4	7	141	140	9	2	71	68																								
6	4	27	29					4	8	40	39	9	3	47	43																								
6	5	170	163					4	9	27	26	9	4	68	68																								
6	6	97	86					4	11	57	55	9	5	29	26																								
6	7	74	73					4	12	67	66	9	7	55	54																								
6	8	70	58					4	13	50	48	9	8	116	124																								
6	9	88	82					4	15	62	60	9	9	66	64																								
6	10	64	62					4	16	42	44	9	10	51	53																								
6	12	168	162					5	1	26	20	9	11	51	52																								
6	13	31	34					5	2	29	27	9	12	51	52																								
6	14	37	34					5	3	49	46	10	1	95	92																								
6	17	73	71					5	4	80	78	10	2	72	73																								
7	1	44	46					5	5	28	17	10	4	47	37																								
7	4	28	27					5	6	93	85	10	6	85	85																								
7	8	85	81					5	7	32	31	10	9	39	38																								
7	9	214	212					5	8	118	115	10	10	41	47																								
7	10	45	42					5	10	90	85	11	2	101	97																								
7	11	27	35					5	11	49	44	11	8	56	52																								
7	12	87	88					5	12	60	58	12	1	59	59																								
7	13	68	65					5	13	86	88	12	3	66	75																								
7	15	43	48					5	14	66	65	12	5	49	51																								

Table E. (concluded)

K	L	FO	FC	K	L	FO	FC
5	6	93	98	8	6	84	91
5	7	50	46	1	1	44	39
5	10	55	50	1	5	55	59
5	11	45	31	1	7	54	40
5	6	93	89	2	2	56	62
6	2	35	16	2	4	37	36
6	3	44	54	2	6	47	48
6	8	64	62	3	3	45	34
6	10	69	69	4	2	55	50
7	3	38	32	4	3	120	115
7	4	65	55	4	4	53	49
7	5	74	78	4	6	49	48
7	7	50	45	5	2	48	55
7	8	52	50	5	3	39	30
8	2	49	42	6	1	52	51
8	3	56	56				
8	5	66	65			M= 14	
8	7	71	70				
9	2	64	55				
		M= 12		8	2	86	89
				1	1	52	47
				2	2	38	33
0	2	153	165				
0	4	45	40				
0	8	81	86				
1	2	63	69				
1	6	89	97				
1	9	67	71				
2	1	97	98				
2	3	47	44				
2	9	58	59				
3	2	49	46				
3	4	53	46				
3	5	67	59				
3	6	58	44				
3	7	52	48				
3	8	43	34				
4	4	52	40				
4	6	45	48				
4	7	76	77				
4	8	73	69				
4	9	76	76				
5	2	56	53				
6	1	45	40				
6	5	60	59				
6	7	43	33				
7	1	75	67				
7	2	63	52				
7	3	42	39				
7	5	58	68				
8	1	47	47				
8	3	103	95				
		M= 13					
8	4	81	81				

Table F. Observed (FO) and Calculated (FC) Structure Factors for Cu₂(Dapac)(OAc).

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
H=-14				1	5	34	33	1	9	34	32	9	2	10	10	8	1	33	33	2	7	23	24	8	3	13	13	3	6	15	15
				1	6	22	21	1	10	10	9	9	3	10	17	6	2	33	34	2	8	30	29	8	5	15	15	3	7	85	86
0	2	58	60	1	7	15	14	1	11	11	10	9	4	25	25	6	4	44	45	2	9	7	7	8	6	31	32	3	8	14	14
0	4	17	17	1	8	50	48	2	1	20	21	9	5	23	23	6	6	7	7	2	10	13	12	8	7	14	14	3	9	14	13
0	6	30	29	1	9	16	14	2	2	23	23	6	7	18	17	6	7	18	17	2	11	9	8	8	8	17	16	3	10	8	7
1	2	9	8	1	10	19	18	2	3	25	26	6	8	38	37	2	12	40	38	3	12	40	38	8	9	8	8	3	11	33	33
1	4	7	5	2	1	21	22	2	4	35	35	6	10	27	26	3	1	24	23	3	1	24	23	8	10	14	13	3	13	34	33
2	2	17	17	2	2	15	15	2	6	29	30	7	1	17	17	3	2	55	55	3	2	55	55	9	1	9	8	4	1	58	59
2	3	32	32	2	4	21	20	2	7	23	22	8	4	13	13	7	2	11	11	3	3	51	53	9	2	11	11	4	2	49	49
2	4	10	11	2	5	17	16	2	8	15	14	8	6	72	73	7	3	24	24	3	4	48	48	9	3	11	13	4	3	16	16
2	5	44	43	2	9	11	10	2	9	13	12	0	10	28	26	7	4	21	21	3	6	54	56	9	6	22	22	4	4	26	26
H=-13				3	1	27	28	2	10	17	16	0	12	18	17	7	5	19	20	3	7	14	15	9	7	14	15	4	5	12	14
				3	2	19	18	3	2	25	26	1	1	12	11	7	6	16	14	3	8	39	39	9	8	12	12	4	7	23	24
				3	3	31	31	3	4	17	17	1	2	20	29	7	7	6	7	3	9	20	20	10	1	19	18	4	8	6	5
8	1	24	25	3	5	47	48	3	5	24	28	1	3	9	9	7	8	6	6	3	10	13	13	10	2	17	16	4	9	25	24
8	3	26	25	3	7	29	28	3	6	25	24	1	4	7	8	7	9	9	9	3	12	15	14	10	4	29	29	4	11	15	15
8	7	39	38	3	9	19	19	3	10	23	21	1	5	31	32	8	1	36	36	4	1	25	25	10	5	16	16	4	13	8	7
8	9	24	23	4	1	29	28	3	11	12	11	1	6	28	28	8	5	45	46	4	3	9	9	10	6	12	12	5	1	7	6
1	1	40	42	4	2	7	5	4	1	28	27	1	9	22	20	8	7	38	38	4	4	8	10	11	3	23	23	5	2	51	50
1	3	44	44	4	3	16	17	4	2	9	7	2	1	42	42	9	1	34	34	4	5	14	13	11	4	10	10	5	4	68	69
1	4	23	22	4	4	7	6	4	3	31	30	2	2	37	36	9	2	20	21	4	6	31	32	11	5	21	21	5	5	21	21
1	5	10	10	4	7	6	5	4	4	24	24	2	4	24	24	9	3	7	7	4	8	19	18	5	6	21	22	5	6	21	22
1	6	12	11	4	8	6	2	4	5	10	9	2	5	33	34	9	4	7	9	4	9	24	23	5	7	14	14	5	7	14	14
1	7	17	17	4	9	13	12	4	6	29	29	2	6	21	22	9	6	18	19	4	10	13	12	0	2	47	46	5	8	58	59
1	9	14	14	5	2	53	54	4	7	9	10	2	7	42	43	9	7	9	9	4	11	18	17	0	4	81	80	5	9	7	7
2	1	11	12	5	3	12	11	4	8	13	12	2	8	20	19	10	1	7	5	4	12	22	20	0	6	24	26	5	10	45	44
2	4	34	32	5	4	30	28	4	9	18	17	2	9	12	12	10	2	15	16	5	1	20	20	0	10	13	13	5	12	14	14
2	6	29	30	5	5	13	13	4	10	11	10	2	10	14	12	10	3	14	13	5	2	16	17	1	1	42	42	6	1	6	2
2	7	11	12	5	6	8	8	5	1	17	16	2	11	31	29	10	4	25	25	5	3	62	62	1	2	85	81	6	2	54	55
2	8	8	8	5	8	36	34	5	2	22	22	3	1	38	37	10	5	17	18	5	4	18	18	1	3	24	24	6	3	16	17
3	2	7	7	6	1	12	12	5	3	16	16	3	2	28	29	3	6	12	12	5	5	33	35	1	4	89	91	6	4	37	38
3	4	32	34	6	2	14	14	5	4	28	29	3	3	12	12	3	7	8	7	5	6	12	12	1	5	32	35	6	5	13	15
3	5	11	11	6	3	18	18	5	5	8	4	3	4	8	7	3	8	7	7	5	7	18	17	1	6	27	26	6	6	17	18
3	6	29	29	6	4	11	10	5	6	7	7	3	5	23	24	0	1	33	34	5	8	13	13	1	7	67	71	6	7	15	16
4	1	13	13	6	7	19	18	5	7	17	17	3	6	17	18	0	3	15	15	5	9	33	33	1	8	62	64	6	8	15	14
4	2	14	14	6	8	14	13	5	8	18	17	3	7	7	7	8	5	36	36	5	10	17	17	1	9	6	6	6	11	7	7
4	3	13	13	7	1	35	34	5	9	24	23	3	12	12	10	8	9	65	64	5	11	7	7	1	10	52	51	7	1	30	31
4	4	23	23	7	2	28	27	5	10	17	16	4	1	22	23	0	11	27	26	6	2	16	15	1	11	24	24	7	2	33	34
4	6	18	18	7	3	10	10	6	1	40	40	4	2	30	29	0	13	22	21	6	3	13	13	1	12	14	14	7	4	26	26
4	7	20	20	7	4	7	7	6	3	48	49	4	3	6	7	1	1	32	31	6	4	18	19	1	13	16	15	7	5	31	31
5	1	29	30	7	5	34	33	6	4	16	15	4	4	6	7	1	2	48	48	6	5	20	20	2	1	75	74	7	7	44	43
5	2	10	10	7	6	17	16	6	5	8	8	4	5	32	32	1	3	97	97	6	6	9	9	2	2	25	25	7	8	27	25
5	3	32	31	6	7	24	23	6	7	24	23	4	6	13	12	1	4	26	25	6	7	18	18	2	3	22	22	7	10	24	24
6	3	14	14	6	9	19	18	6	9	19	18	4	7	34	34	1	5	28	28	6	8	9	10	2	4	8	9	7	11	26	23
H=-11				7	1	15	15	7	1	15	15	4	8	31	30	1	6	65	65	6	9	31	30	2	5	28	29	8	1	30	29
				7	2	19	18	7	2	19	18	4	10	16	14	1	7	19	19	6	11	16	15	2	6	29	31	8	2	16	18
				7	3	7	6	7	3	7	6	4	12	26	24	1	8	21	21	7	1	11	11	2	7	13	18	8	5	9	18
				7	5	24	24	7	5	24	24	5	1	26	26	1	9	19	30	7	2	15	16	2	8	15	14	8	6	26	27
				7	6	29	28	7	6	29	28	5	2	29	29	1	10	29	28	7	3	24	24	2	9	13	16	8	7	8	6
				7	7	22	22	7	7	22	22	5	3	24	23	1	11	12	11	7	4	33	34	2	10	6	5	8	8	19	19
				7	8	11	11	7	8	11	11	5	4	17	17	2	1	19	19	7	5	32	32	2	11	18	18	9	1	23	22
				8	2	10	10	8	2	10	10	5	5	6	6	2	2	11	10	7	6	25	26	2	12	13	12	9	3	8	8
				8	4	31	36	8	4	31	36	5	7	12	11	2	3	51	51	7	9	7	6	3	1	104	102	9	4	7	8
				1	6	21	21	8	5	15	15	5	8	8	9	2	4	16	16	7	10	21	20	3	2	13	14	9	5	34	35
				1	7	37	36	8	6	27	27	5	9	13	13	2	5	11	10	8	1	30	30	3	4	28	28	9	6	22	22
				1	8	8	9	9	1	14	14	5	10	7	6	2	6	51	52	8	2	14	13	3	5	77	78	9	7	23	22

Table F. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC						
9	8	15	15	4	3	82	87	10	4	8	8	4	1	81	88	8	11	21	20	2	4	13	14	7	2	74	75	M = -4									
10	1	14	14	4	5	41	42	10	5	19	21	4	2	37	34	9	1	43	44	2	5	11	9	7	3	35	36	0	2	16	16	0	4	77	83		
10	2	40	39	4	6	48	49	10	6	16	16	4	3	14	16	9	2	11	9	2	7	12	14	7	4	10	9	0	8	48	48	0	8	6	7		
10	3	22	22	4	7	5	5	10	9	26	25	4	4	71	73	9	3	43	45	2	8	32	33	7	5	57	58	0	8	45	45	0	8	45	45		
10	5	16	16	4	8	53	55	11	1	8	7	4	5	25	26	9	4	20	21	2	9	33	33	7	6	50	52	0	10	50	61	1	1	34	45		
10	6	8	8	4	9	38	39	11	2	14	15	4	6	65	66	9	5	9	9	2	10	26	26	7	8	45	45	0	8	45	45	1	1	34	45		
10	8	12	12	4	10	7	7	11	3	6	6	4	7	59	61	9	6	14	13	2	11	6	5	7	9	15	15	0	10	50	61	1	1	34	45		
11	1	8	8	4	11	10	9	11	4	29	30	4	8	24	24	9	7	21	22	2	12	19	17	7	11	32	31	1	1	34	45	1	1	34	45		
11	2	12	13	4	12	15	16	11	5	15	15	4	9	24	25	9	8	29	29	2	13	11	11	7	12	18	17	1	2	31	34	1	5	5	5		
11	3	10	11	5	2	35	34	11	6	11	12	4	10	25	25	9	9	13	13	2	14	29	27	8	1	48	48	1	4	35	45	1	5	5	5		
11	4	28	28	5	3	26	27	12	2	10	10	4	11	29	29	10	1	17	10	3	1	16	14	8	2	25	26	1	6	47	50	1	7	21	22		
12	1	14	13	5	4	34	34	12	3	16	17	4	12	28	27	10	2	16	15	3	2	172	168	8	3	33	34	1	6	47	50	1	8	11	10		
12	3	24	24	5	5	33	33	12	4	9	9	4	13	29	29	10	3	14	14	3	3	32	33	8	4	6	7	1	7	21	22	1	9	30	29		
M = -7				5	8	22	22	12	5	18	18	5	1	24	23	10	4	40	42	3	4	10	19	8	5	15	14	1	8	11	10	1	9	30	29		
				5	9	31	32	M = -6				5	2	35	36	10	5	49	51	3	5	9	10	8	7	32	33	1	9	30	29	1	10	43	43		
				5	10	22	22	0	2	81	78	5	3	44	43	10	6	34	34	3	6	111	119	8	8	13	14	1	10	43	43	1	12	32	31		
0	1	15	17	5	11	28	28	0	4	58	63	5	4	53	54	10	7	17	17	3	7	24	25	8	9	21	22	1	12	32	31	2	1	106	115		
0	3	127	140	6	2	20	19	0	5	20	22	5	5	20	22	11	1	6	6	3	8	72	77	8	12	22	21	1	13	31	31	2	2	14	14		
0	5	83	87	6	3	87	86	0	6	44	43	5	6	27	26	11	2	19	19	3	9	28	29	9	1	25	25	2	3	34	45	2	3	34	45		
0	9	71	71	6	4	11	11	0	8	52	53	5	7	22	23	11	3	16	18	3	10	15	16	9	2	50	50	2	2	14	14	2	3	34	45		
0	11	23	22	6	5	57	60	0	10	50	51	5	8	28	19	11	4	24	24	3	12	33	31	9	3	11	12	2	4	33	35	2	5	40	41		
0	13	8	6	6	6	6	7	0	12	32	32	5	9	21	21	11	5	20	21	3	14	25	24	9	4	11	12	2	4	33	35	2	7	61	66		
1	1	5	3	6	7	6	7	0	14	29	29	5	10	7	8	11	6	14	15	4	2	63	64	9	5	33	35	2	5	40	41	2	9	25	25		
1	2	11	10	6	8	9	9	0	16	29	29	5	12	9	11	12	1	21	21	4	3	78	78	9	6	43	46	2	7	61	66	2	10	15	16		
1	4	12	13	6	9	36	37	1	1	56	83	6	1	38	29	12	2	29	29	4	4	13	13	9	8	30	30	2	9	25	25	2	11	25	25		
1	5	19	19	6	10	13	12	1	2	17	15	6	2	50	51	12	3	32	33	4	5	28	29	9	9	20	20	2	10	15	16	2	11	25	25		
1	6	22	22	6	11	31	31	1	3	44	44	6	3	30	29	12	4	28	29	4	6	14	14	9	10	16	15	2	11	25	25	2	12	11	11		
1	7	29	29	7	1	57	57	1	4	52	57	6	4	75	79	13	1	23	23	4	7	33	33	9	11	8	7	2	12	11	11	2	14	8	7		
1	8	15	16	7	2	10	11	1	6	41	41	6	5	16	17	13	2	10	10	4	8	20	21	10	1	15	16	3	1	34	36	3	2	38	48		
1	9	47	48	7	3	10	10	1	7	28	29	6	6	27	28	13	3	25	25	4	10	6	7	10	2	15	15	3	1	34	36	3	3	80	85		
1	11	28	29	7	4	9	8	1	9	15	16	6	7	34	35	13	4	22	23	4	11	19	19	10	3	28	30	3	2	38	48	3	4	42	39		
1	12	26	25	7	5	24	25	1	11	16	17	6	8	22	23	13	5	15	15	4	12	25	25	10	4	39	41	3	3	80	85	3	4	42	39		
1	13	15	13	7	6	28	28	1	14	8	7	6	9	19	18	13	6	12	12	5	13	15	15	10	5	11	13	3	4	42	39	3	6	27	26		
1	14	11	11	7	7	23	24	2	1	92	98	6	10	52	53	13	7	11	11	5	1	20	22	10	6	28	29	3	7	113	117	3	8	8	9		
2	1	11	8	7	8	27	27	2	2	6	2	6	11	6	7	13	8	12	14	5	2	9	11	10	7	16	17	3	7	113	117	3	9	41	40		
2	2	106	110	7	9	24	23	2	3	39	39	6	12	19	19	13	9	15	15	5	3	91	97	10	10	26	24	3	8	8	9	3	10	13	13		
2	3	48	46	7	10	14	14	2	4	39	43	7	1	72	71	13	10	14	14	5	4	15	14	11	2	10	11	3	9	41	40	3	11	10	11		
2	4	9	9	7	12	13	13	2	5	16	18	7	2	22	22	13	11	13	12	5	5	98	106	11	3	38	39	3	10	13	13	3	11	10	11		
2	5	36	37	8	1	12	11	2	7	93	95	7	3	19	19	13	12	12	12	5	6	21	20	11	4	14	14	3	12	7	8	4	13	12	11		
2	6	76	80	8	2	36	36	2	8	42	43	7	4	43	44	1	1	31	32	5	7	18	18	11	5	42	43	3	12	7	8	4	14	12	11		
2	8	59	60	8	4	10	11	2	9	33	32	7	5	25	27	1	2	64	65	5	8	22	23	11	6	6	5	3	13	42	41	4	1	131	124		
2	9	17	18	8	6	44	44	2	10	23	25	7	6	43	46	1	3	84	87	5	9	66	69	11	7	7	8	4	1	131	124	4	2	41	41		
2	10	7	7	8	8	34	35	2	11	8	8	7	7	13	13	1	4	8	7	5	10	17	17	11	9	17	17	4	2	41	41	4	3	21	24		
2	11	13	12	8	10	9	9	2	13	46	44	7	8	6	5	1	5	46	55	5	11	34	34	12	1	18	19	4	3	21	24	4	4	117	126		
2	12	19	19	8	11	18	9	3	14	10	9	7	10	7	6	1	6	27	30	5	12	15	15	12	2	12	14	4	5	23	23	4	6	5	3		
3	1	47	47	9	2	15	15	3	1	154	156	7	11	18	18	1	7	12	13	6	1	34	33	12	3	6	7	4	5	23	23	4	7	25	26		
3	4	7	8	9	3	9	10	3	2	42	39	7	12	13	13	1	8	49	53	6	2	12	13	12	4	33	36	4	6	5	3	4	33	34			
3	5	53	53	9	4	34	34	3	3	83	82	8	1	42	42	1	9	59	61	6	3	14	15	12	6	11	11	4	7	25	26	4	8	39	40		
3	6	46	47	9	5	22	23	3	4	5	6	8	2	38	40	1	10	8	7	6	4	51	54	12	7	17	19	4	8	33	34	4	10	39	40		
3	7	18	20	9	6	23	23	3	5	31	31	8	3	20	20	1	11	16	17	6	5	13	14	13	1	21	21	4	13</								

Table F. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
5	5	32	34	10	8	26	25	2	12	13	12	7	4	15	17	H = -2				5	3	5	9	10	9	14	13	2	12	7	7				
5	6	73	75	10	9	13	13	2	13	19	19	7	5	28	28					5	4	71	77	10	10	16	16	2	14	18	18				
5	7	41	43	11	1	9	9	2	14	28	27	7	6	28	28	0				5	6	65	68	11	1	28	28	3	1	129	128				
5	8	7	8	11	2	5	5	3	1	33	35	7	7	33	33	0				5	8	19	19	11	2	29	32	3	2	141	143				
5	9	24	24	11	3	38	31	3	2	48	52	7	8	7	5	0				5	9	12	12	11	3	13	13	3	3	5	8				
5	10	56	56	11	4	14	15	3	3	10	13	7	9	19	19	0				5	10	19	19	11	4	29	29	3	4	139	142				
5	11	6	6	11	5	27	29	3	4	21	22	7	10	8	9	0				5	11	31	31	11	5	26	26	3	5	43	42				
5	12	32	32	11	6	26	26	3	6	6	7	7	11	11	11	0				5	12	8	7	11	6	28	28	3	7	5	4				
6	1	46	48	11	7	7	6	3	7	35	36	8	1	12	11	1				6	1	88	88	11	7	22	23	3	8	115	118				
6	2	27	26	11	8	6	5	3	8	32	33	8	2	76	82	1				6	2	61	66	12	1	19	19	3	9	19	19				
6	4	60	62	11	9	11	10	3	9	7	7	8	3	26	27	1				6	4	63	65	12	2	17	20	3	10	47	48				
6	5	25	25	12	1	22	23	3	10	9	8	8	4	25	26	1				6	5	53	52	12	3	16	16	3	12	18	18				
6	6	36	36	12	4	15	16	3	11	11	11	8	6	8	7	1				6	6	62	62	12	4	32	31	3	14	31	32				
6	7	23	23	12	5	23	24	3	12	20	20	8	7	13	13	1				6	8	31	31	12	5	24	24	4	1	69	78				
6	8	23	24	12	6	14	15	3	13	7	9	8	8	26	28	1				6	9	37	37	12	6	12	12	4	2	33	29				
6	9	5	4	12	7	20	21	3	14	30	30	8	9	14	13	1				6	10	45	44	12	7	11	11	4	3	5	6				
6	11	23	22	13	1	6	5	4	1	81	81	8	10	25	25	1				6	11	27	27	13	1	22	23	4	4	25	22				
7	1	26	28	13	2	33	33	4	2	115	117	8	11	7	7	1				6	12	29	29	13	2	15	15	4	5	19	19				
7	2	29	30	13	3	16	17	4	3	43	44	9	1	50	50	1				6	13	6	4	13	3	22	22	4	6	50	50				
7	3	43	44	13	4	12	14	4	4	12	14	9	2	21	22	1				7	1	86	89	13	4	16	16	4	7	5	4				
7	4	47	49	13	5	8	8	4	5	101	104	9	3	51	55	2				7	2	6	7	13	6	7	6	4	9	26	26				
7	5	29	31	13	6	16	15	4	6	51	49	9	4	33	36	2				7	3	76	79	14	1	17	15	4	11	19	19				
7	6	18	18					4	7	28	28	9	5	21	21	2				7	4	23	22	14	2	22	23	4	13	20	21				
7	7	37	38					4	8	70	71	9	6	24	26	2				7	5	22	21	14	3	8	8	5	1	84	98				
7	8	17	17					4	9	45	45	9	7	12	11	2				7	6	30	30					5	2	89	85				
7	9	8	8					4	10	28	29	9	8	28	26	2				7	7	43	43					5	3	6	7				
7	10	23	22					4	11	37	36	9	11	7	6	2				7	8	39	38					5	4	18	24				
7	11	7	8					4	12	8	6	10	1	25	25	2				7	9	20	21					5	5	119	119				
7	12	16	16					4	14	14	14	10	2	17	17	2				7	12	16	16					5	7	76	77				
8	1	82	81					5	1	32	28	10	3	20	21	2				8	1	17	16					5	8	16	16				
8	2	15	15					5	2	14	10	10	4	27	28	2				8	2	38	42					5	10	5	5				
8	3	14	15					5	3	51	54	10	5	32	33	2				8	3	20	20					5	11	53	54				
8	4	12	12					5	4	5	5	10	7	15	15	2				8	4	32	31					5	13	29	28				
8	5	8	8					5	5	26	26	10	8	13	13	3				8	5	7	8					6	1	68	71				
8	6	18	18					5	6	30	31	10	9	22	22	3				8	6	12	10					6	2	181	99				
8	7	19	19					5	7	18	18	10	10	9	10	3				8	7	40	40					6	3	47	46				
8	8	27	26					5	8	12	12	11	1	29	29	3				8	8	16	16					6	4	27	27				
8	9	8	6					5	10	7	8	11	2	5	5	3				8	9	31	32					6	5	5	5				
8	10	11	11					5	11	48	38	11	3	10	10	3				8	10	12	11					6	6	36	36				
8	12	8	9					5	12	19	19	11	4	41	44	3				8	11	20	21					6	7	14	13				
9	1	24	23					5	13	15	14	11	6	32	32	3				9	1	32	32					6	8	9	9				
9	2	54	56					6	1	25	27	11	7	7	6	3				9	2	38	40					6	9	21	21				
9	3	14	14					6	2	17	17	12	1	11	11	4				9	3	69	71					6	10	30	30				
9	4	11	13					6	3	48	51	12	2	20	21	4				9	4	24	25					6	11	17	17				
9	5	16	16					6	4	40	41	12	3	15	16	4				9	5	46	47					6	12	24	24				
9	6	28	28					6	5	95	99	12	4	16	16	4				9	7	18	17					6	13	8	7				
9	7	23	24					6	6	14	16	12	5	24	24	4				9	9	28	28					7	1	64	69				
9	8	6	5					6	7	29	30	12	6	19	19	4				9	10	21	20					7	2	72	72				
9	9	11	11					6	8	26	27	12	7	9	9	4				9	11	9	9					7	3	42	41				
9	10	8	6					6	9	32	33	12	8	16	17	4				10	1	19	19					7	4	85	84				
9	11	8	7					6	11	22	22	13	1	18	18	4				10	2	14	14					7	5	47	47				
10	1	9	9					6	12	11	10	13	2	11	13	4				10	3	12	12					7	6	12	14				
10	2	36	37					6	13	22	22	13	3	43	46	4				10	4	5	4					7	8	75	76				
10	3	31	32					7	1	41	40	13	4	8	8	4				10	5	8	10					7	9	8	9				
10	4	31	34					7	2	48	50	13	6	8	5	5				10	6	36	35					7	10	32	32				
10	5	22	23					7	3	10	12	14	2	25	26	5				10	7	26	25					7	11	30	30				

Table F. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
0	1	15	16	0	10	35	35	5	4	40	38	10	2	22	22	2	11	19	20	7	9	17	17								
0	2	54	54	0	12	16	16	5	5	43	43	10	3	46	45	2	12	10	10	7	11	19	20								
0	3	50	51	1	1	6	4	5	6	68	59	10	4	32	31	2	13	21	22	7	12	9	9								
0	4	16	15	1	2	24	20	5	7	40	40	10	5	10	17	3	0	101	99	8	0	7	5								
0	5	16	15	1	3	150	146	5	8	34	33	10	6	35	35	3	1	30	27	8	1	25	25								
0	6	7	7	1	4	7	12	5	9	10	11	10	6	6	6	3	2	138	122	8	2	69	65								
0	7	32	33	1	5	9	11	5	10	11	10	10	9	15	15	3	3	61	56	8	3	58	52								
0	9	30	30	1	6	127	125	5	11	11	10	10	10	14	14	3	4	79	77	8	4	69	65								
0	10	16	15	1	7	47	49	5	12	49	50	11	1	31	31	3	5	10	7	8	5	11	10								
9	1	43	45	1	8	21	20	5	13	11	12	11	4	10	11	3	6	46	46	8	6	7	8								
9	2	73	71	1	9	31	32	6	0	111	120	11	5	36	35	3	7	19	19	8	7	7	7								
9	4	47	46	1	10	29	28	6	1	75	70	11	6	35	35	3	8	15	17	8	8	46	45								
9	5	26	25	1	11	10	19	6	2	88	85	11	7	27	27	3	9	7	6	8	10	31	31								
9	6	6	5	1	12	36	35	6	3	28	27	11	8	7	7	3	11	6	7	9	0	10	10								
9	7	32	32	1	13	17	17	6	4	47	40	12	0	31	33	4	0	81	60	9	1	10	8								
9	8	58	57	1	14	14	13	6	5	6	6	12	2	11	9	4	1	92	89	9	2	27	27								
9	9	6	5	2	0	88	99	6	6	82	82	12	3	20	19	4	2	73	69	9	3	52	48								
9	10	32	33	2	1	178	170	6	7	38	37	12	4	16	16	4	3	18	20	9	4	30	28								
9	11	16	16	2	2	145	139	6	8	26	26	12	5	18	18	4	4	24	29	9	5	32	31								
10	1	24	23	2	3	257	236	6	9	22	23	12	6	8	8	4	5	51	50	9	6	6	6								
10	2	10	9	2	4	5	7	6	10	12	11	13	1	7	7	4	6	12	10	9	7	12	13								
10	3	9	9	2	5	112	109	6	11	4	9	13	2	36	35	4	7	56	54	9	8	32	32								
10	4	45	45	2	6	84	84	6	12	16	17	13	3	17	18	4	8	59	60	9	10	4	7								
10	5	12	11	2	7	70	70	7	1	21	20	13	4	37	36	4	10	45	45	10	0	44	45								
10	6	20	20	2	8	19	19	7	2	43	40	13	5	13	13	4	11	29	28	10	1	44	43								
10	7	6	7	2	9	25	25	7	3	36	34	14	0	19	19	4	13	18	17	10	2	52	50								
10	8	12	11	2	11	5	4	7	4	52	50	14	1	11	11	5	0	18	18	10	3	19	19								
10	9	14	13	2	13	7	6	7	5	63	60	14	2	26	24	5	1	77	77	10	5	33	32								
10	10	14	13	3	1	124	109	7	6	31	30					5	2	23	20	10	6	14	15								
11	1	29	30	3	2	14	12	7	7	6	6					5	3	4	3	10	7	31	30								
11	4	8	8	3	3	28	26	7	8	9	10					5	4	82	75	10	8	14	14								
11	5	49	47	3	4	38	35	7	9	36	36	0	1	267	263	5	5	35	36	11	0	12	11								
11	6	14	13	3	5	7	7	7	10	34	34	0	3	91	79	5	6	24	24	11	1	12	12								
11	7	35	34	3	6	67	66	7	11	19	20	0	5	127	126	5	7	27	26	11	2	25	24								
11	9	10	12	3	7	53	54	7	12	19	20	0	7	85	87	5	8	24	24	11	5	12	11								
12	1	26	26	3	8	10	10	8	1	50	49	0	11	50	50	5	9	20	19	11	6	33	32								
12	2	21	20	3	9	67	68	8	2	19	17	0	13	37	38	5	12	14	14	11	7	8	6								
12	3	22	22	3	11	18	18	8	3	103	101	1	0	11	13	6	0	25	27	11	8	17	15								
12	4	18	17	3	13	26	26	8	5	21	21	1	1	166	157	6	1	50	51	12	0	18	19								
12	5	7	6	4	0	284	215	8	7	33	33	1	2	71	73	6	2	21	19	12	1	17	16								
12	6	24	23	4	1	62	61	8	8	26	27	1	3	23	19	6	4	60	58	12	2	9	7								
12	7	13	11	4	2	24	23	8	9	32	31	1	4	18	15	6	5	98	94	12	3	29	28								
13	1	18	17	4	3	108	105	8	10	14	13	1	5	11	15	6	6	43	40	12	4	18	17								
13	2	30	29	4	4	29	28	8	11	9	10	1	6	42	39	6	7	67	65	12	5	20	19								
13	3	23	21	4	5	74	71	9	1	20	20	1	7	17	17	6	9	8	8	12	6	19	19								
13	4	20	19	4	6	107	106	9	2	68	56	1	8	16	17	6	10	18	17	12	7	10	10								
13	5	14	14	4	7	14	12	9	3	36	34	1	9	9	7	6	11	40	40	13	0	10	10								
14	1	10	10	4	8	9	9	9	4	32	30	2	0	12	9	7	0	9	10	13	1	19	19								
14	3	33	31	4	9	41	42	9	5	6	5	2	1	11	4	7	1	72	67	13	2	19	17								
				4	10	37	37	9	6	26	27	2	2	41	49	7	2	85	84	13	3	26	25								
				4	11	7	8	9	7	31	32	2	3	18	16	7	3	32	33	13	5	12	11								
				4	12	9	8	9	8	37	36	2	4	129	128	7	4	9	8	14	1	28	18								
0	2	96	90	4	13	8	7	9	9	33	33	2	5	70	69	7	5	21	20	14	2	17	16								
0	4	125	125	5	1	59	55	9	10	10	11	2	7	40	39	7	6	33	31	14	3	15	15								
0	6	162	155	5	2	4	3	10	0	50	55	2	8	67	67	7	7	12	11												
0	8	44	47	5	3	9	8	10	1	10	10	2	10	38	38	7	8	36	37												

Table F. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	
10	7	21	28	3	1	30	30	8	5	40	39	1	6	28	28	6	6	67	65	M= 5	5	7	27	26	12	3	7	2	12	3	7	2
10	9	10	10	3	2	40	38	8	6	10	10	1	7	10	11	6	7	27	28	0	1	81	77	5	9	12	13	13	4	7	6	
11	0	45	46	3	3	39	35	8	7	7	7	1	8	43	43	6	8	58	56	0	5	53	49	5	10	8	7	13	2	8	6	
11	1	21	19	3	4	101	97	8	8	15	15	1	9	17	16	6	9	16	16	0	3	113	104	6	1	69	67	M= 6	0	11	1	0
11	2	23	22	3	5	32	30	8	9	30	31	1	10	9	11	6	10	12	14	0	9	32	33	6	0	42	40	6	2	31	30	
11	3	9	8	3	6	32	32	8	10	7	8	1	11	20	22	7	0	15	17	0	7	119	120	6	1	69	67	0	0	11	1	0
11	6	24	25	3	8	34	35	9	1	17	17	1	12	35	37	7	1	34	33	0	9	32	33	6	2	31	30	1	1	12	14	0
11	7	21	21	3	9	18	18	9	2	47	45	2	0	91	88	7	2	13	11	0	11	12	14	6	3	39	30	0	0	11	1	0
11	8	20	20	3	10	12	62	9	3	47	46	2	2	69	63	7	3	56	51	1	0	126	116	6	4	26	28	8	2	65	63	0
12	0	8	9	3	12	25	25	9	4	62	60	2	3	87	83	7	4	37	36	1	1	171	158	6	5	31	31	0	4	28	28	0
12	1	27	26	4	0	61	61	9	5	12	11	2	4	18	17	7	5	23	23	1	2	15	14	6	6	15	14	0	6	63	64	0
12	2	21	19	4	1	117	109	9	6	10	11	2	5	138	125	7	6	24	24	1	3	52	51	6	7	45	45	1	0	130	120	0
12	3	13	11	4	2	38	35	9	7	22	23	2	6	42	41	7	8	10	10	1	4	93	89	6	9	30	31	1	1	58	58	0
12	4	34	32	4	3	5	7	9	8	22	22	2	8	37	36	7	9	19	22	1	5	6	8	6	10	7	6	1	2	115	114	0
12	5	14	15	4	4	14	16	9	9	10	8	2	9	44	44	7	10	19	19	1	6	47	47	7	0	49	40	1	3	46	46	0
12	7	24	23	4	5	9	10	10	0	24	24	2	11	34	34	8	0	12	10	1	7	49	47	7	1	16	15	1	4	39	38	0
13	0	7	7	4	6	21	22	10	1	70	69	2	12	10	10	8	1	8	8	1	6	13	13	7	2	25	25	1	5	84	82	0
13	1	7	7	4	7	43	43	10	2	34	34	3	0	79	68	8	3	62	58	1	11	11	11	7	3	55	54	1	6	45	45	0
13	2	23	22	4	12	13	12	10	4	31	31	3	1	4	7	8	5	64	62	2	0	44	40	7	4	22	21	1	7	22	22	0
13	3	27	26	5	0	38	28	10	5	19	19	3	2	33	30	8	6	19	19	2	1	121	109	7	5	19	10	1	8	52	52	0
13	5	10	9	5	1	73	67	10	6	35	34	3	4	27	28	8	8	10	9	2	2	13	9	7	6	6	6	1	9	10	11	0
14	0	11	11	5	2	21	20	10	7	15	15	3	5	15	17	8	9	40	40	2	3	25	22	7	7	6	7	1	10	10	17	0
14	2	23	21	5	3	57	54	10	8	21	21	3	6	24	23	8	10	10	9	2	4	93	89	7	8	12	13	1	11	25	25	0
				5	4	34	34	11	0	44	44	3	7	18	18	9	8	62	61	2	5	44	42	7	9	21	21	2	0	6	7	0
				5	5	31	30	11	1	22	22	3	9	23	23	9	1	7	7	2	6	66	66	8	0	24	20	2	1	44	42	0
				5	6	5	2	11	2	34	33	3	10	15	19	9	3	17	16	2	7	41	40	8	1	14	13	2	2	13	12	0
				5	7	65	63	11	3	10	10	3	11	28	29	9	4	38	37	2	8	8	8	8	2	13	12	2	3	7	7	0
				5	8	30	31	11	4	9	9	3	12	7	6	9	6	16	15	2	9	13	14	8	3	18	17	2	4	41	40	0
				5	9	28	28	11	5	8	8	4	0	104	99	9	7	16	16	2	10	53	53	8	4	44	44	2	6	15	15	0
				5	11	15	16	11	7	37	37	4	1	12	9	9	8	18	18	2	11	14	13	8	5	20	19	2	7	9	10	0
				6	0	32	30	12	0	11	10	4	2	52	53	9	9	29	38	3	0	113	110	8	6	31	31	2	10	14	14	0
				6	1	123	121	12	1	25	24	4	3	86	84	10	0	36	34	3	1	61	55	8	8	14	14	2	11	29	38	0
				6	2	87	82	12	2	14	15	4	4	18	17	10	1	7	8	3	2	23	24	8	9	8	7	3	1	40	39	0
				6	3	42	44	12	3	46	44	4	5	81	79	10	2	51	51	3	3	8	9	9	0	38	39	3	2	21	20	0
				6	4	11	10	12	4	14	14	4	6	69	68	10	3	22	22	3	4	91	86	9	1	24	23	3	3	69	67	0
				6	5	29	29	12	5	12	12	4	7	24	25	10	5	19	19	3	6	78	80	9	2	8	7	3	4	43	40	0
				6	6	11	10	12	6	13	12	4	8	37	38	10	6	32	31	3	7	45	47	9	4	23	23	3	5	130	130	0
				6	7	21	21	13	8	13	13	4	9	23	23	10	7	6	4	3	9	13	11	9	5	20	20	3	7	35	35	0
				6	8	31	31	13	1	9	7	4	10	8	7	10	8	28	28	3	10	6	6	9	7	11	11	3	8	21	22	0
				6	9	10	9	13	3	13	14	4	11	28	30	11	0	19	19	3	11	14	13	9	8	12	12	3	9	29	30	0
				6	11	12	13	13	4	21	21	5	0	91	86	11	1	42	41	4	0	38	37	10	0	6	4	4	8	8	9	0
				7	0	32	32	14	0	19	18	5	1	52	50	11	2	7	5	4	1	29	27	10	1	13	12	4	1	28	30	0
				7	1	45	43					5	2	6	5	11	3	24	24	4	2	42	41	10	2	33	34	4	2	40	37	0
				7	2	25	24	M= 4				5	3	30	29	11	5	11	11	4	3	47	44	10	3	30	32	4	3	10	10	0
				7	4	72	71					5	5	6	6	11	6	9	9	4	4	83	82	10	4	31	31	4	4	18	16	0
				7	5	39	38	0	0	123	126	5	6	17	10	11	7	17	17	4	6	33	33	10	6	9	9	4	5	22	22	0
				7	6	42	42	0	2	142	146	5	7	21	21	12	0	15	14	4	7	52	53	10	7	24	24	4	6	9	9	0
				7	7	51	51	0	4	35	36	5	8	16	16	12	1	9	8	4	8	14	13	11	0	10	9	4	7	25	25	0
				7	8	34	36	0	6	166	162	5	9	15	15	12	2	25	24	4	9	27	27	11	1	36	36	4	8	15	16	0
				7	10	38	39	0	8	67	68	5	11	9	10	12	3	10	9	4	10	23	23	11	2	21	21	4	9	11	11	0
				7	11	12	13	0	12	30	30	6	0	71	68	12	4	11	9	5	0	24	22	11	3	13	13	4	10	14	14	0
				8	0	26	25	1	0	41	33	6	1	20	18	12	5	15	14	5	1	113	118	11	4	10	11	5	0	59	55	0
				8	1	5	3	1	2	28	23	6	2	121	115	13	0	12	12	5	2	21	20	11	6	7	7	5	1	13	11	0
				8	2	57	56	1	3	52	45	6	3	29	20	13	1	12	12	5	3	48	46	12	0	25	24	5	2	116	112	0
				8	3	34	32	1	4	33	31	6	4	11	11	13	2	14	15	5	4	14	14	12	1	13	11	5	3	22	21	0
				8	4	52	52	1	5	10	15	6	5	19	19					5	6	26	25	12	2	24	24	5	4	43	41	0

Table F. (concluded)

Table G. Observed (FO) and Calculated (FC) Structure Factors for $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$.

[illegible]

Table G. (continued)

K	L	FC	FC	K	L	FC	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	FC	FC	K	L	F0	FC				
2	12	32	36	3	12	14	15	4	8	36	31	5	1	29	31	4	3	186	181	3	7	57	56	4	3	113	110	3	7	42	43
2	13	19	19	3	13	21	27	4	9	23	20	5	2	68	68	4	5	51	51	3	8	58	58	4	4	43	45	3	8	82	88
4	1	189	112	5	1	52	51	4	10	36	35	5	3	105	107	4	5	30	29	3	10	55	57	4	5	24	22	3	9	44	44
4	2	83	86	5	2	43	44	4	11	16	16	5	4	17	16	4	6	111	109	3	11	42	43	4	6	23	22	3	10	24	25
4	3	16	15	5	3	77	77	6	1	83	86	5	5	91	92	4	7	82	81	3	12	44	47	4	7	42	42	3	11	34	36
4	4	71	68	5	4	45	46	6	2	63	66	5	6	55	55	4	8	8	8	3	13	9	5	4	8	62	61	3	12	38	48
4	5	69	69	5	5	57	56	6	3	75	78	5	7	66	67	4	10	49	50	5	1	27	24	4	9	22	21	5	1	163	143
4	6	53	51	5	6	39	39	6	5	54	52	5	9	23	25	4	11	38	40	5	2	79	77	4	10	47	47	5	2	44	44
4	7	40	40	5	7	45	44	6	6	29	29	5	10	31	33	4	12	24	26	5	3	12	104	4	11	31	33	5	3	98	98
4	8	39	41	5	8	35	35	6	7	30	31	5	11	22	23	4	13	18	21	5	4	47	46	4	12	24	25	5	4	69	70
4	9	60	63	5	9	42	41	6	9	45	48	5	12	15	17	6	1	26	25	5	6	79	79	6	1	11	13	5	5	45	43
4	10	39	43	5	10	17	19	6	10	9	9	7	1	64	64	6	2	45	45	5	7	68	67	6	2	34	34	5	6	43	45
4	11	12	13	7	1	99	106	6	11	16	18	7	2	33	32	6	3	125	124	5	8	7	9	6	3	158	159	5	7	49	49
4	12	12	14	7	2	75	79	8	1	30	30	7	3	131	137	6	4	36	36	5	10	39	40	6	4	71	69	5	8	46	47
6	1	97	100	7	3	28	28	8	3	53	54	7	4	19	28	6	5	24	22	5	11	34	34	6	5	16	13	5	9	34	32
6	2	47	50	7	4	29	40	8	5	18	18	7	5	44	43	6	7	60	61	5	12	12	13	6	6	26	26	5	10	23	22
6	4	10	11	7	5	12	11	8	6	10	11	7	7	36	38	6	8	11	14	7	2	14	12	6	7	52	52	5	11	37	37
6	5	47	49	7	6	17	18	8	7	47	50	7	9	38	40	6	9	31	33	7	3	149	152	6	8	19	20	5	12	17	21
6	6	22	24	7	7	32	34	8	9	41																					

Table G. (continued)

K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC
2	9	29	20	1	4	162	169	11	3	14	11	8	7	38	36	4	11	19	16	5	0	0	6	4	1	92	85	4	1	92	85
2	10	16	15	1	5	15	15	11	4	25	22	8	8	8	4	4	12	30	26	5	1	148	137	4	2	113	115	4	2	113	115
2	11	19	22	1	6	73	75	11	5	42	39	8	9	29	27	6	0	39	38	5	2	121	113	4	3	61	63	4	3	61	63
2	12	49	50	1	7	34	33	11	6	14	11	8	10	13	12	6	1	103	97	5	3	95	95	4	4	53	53	4	4	53	53
4	0	171	167	1	8	111	107					10	0	16	13	7	6	43	41	6	2	74	70	5	4	70	69	4	5	41	43
4	1	120	123	1	9	23	23					10	1	67	61	7	9	32	30	6	3	23	22	5	5	109	107	4	6	67	69
4	2	72	61	1	10	14	16					10	2	7	9	7	11	11	10	6	5	111	109	5	6	45	45	4	7	30	32
4	3	23	24	1	11	20	18					10	3	18	16	9	1	49	46	6	6	47	46	5	7	25	25	4	8	16	12
4	4	109	111	1	12	51	49					10	4	12	12	9	3	9	9	6	8	22	21	5	8	26	25	4	9	26	28
4	5	107	103	3	0	163	152					10	5	44	41	9	4	17	17	6	9	28	27	5	9	27	26	4	10	25	26
4	6	17	14	3	1	12	6					10	6	13	10	9	5	49	46	8	0	8	10	5	10	22	23	4	11	25	24
4	7	31	29	3	2	23	19					10	7	25	22	9	6	16	15	8	1	63	62	5	11	27	26	6	1	63	60
4	8	81	80	3	3	35	32					12	0	29	27	9	7	15	13	8	2	11	8	5	12	17	13	6	2	54	53
4	9	59	59	3	4	102	100					12	1	32	29	9	9	32	29	8	3	9	6	7	0	20	18	6	3	66	64
4	10	23	21	3	5	40	43					12	2	11	9	11	0	17	15	8	5	63	61	7	1	61	61	6	4	20	17
4	11	22	24	3	6	48	47									11	1	55	54	8	6	10	8	7	2	34	32	6	5	82	82
4	12	34	35	3	7	96	96									11	2	25	22	8	7	9	8	7	3	45	46	6	6	29	30
4	13	12	12	3	8	28	90									11	3	9	10	8	9	35	34	7	5	93	92	6	7	59	58
6	0	117	108	3	9	39	39					1	0	145	144	11	4	20	17	10	1	46	42	7	6	25	25	6	8	15	14
6	1	89	87	3	11	17	19					1	1	108	113	11	5	49	44	10	2	16	13	7	7	39	37	6	9	41	41
6	2	11	12	3	12	42	43					1	2	133	138	11	6	15	13	10	3	9	10	7	8	22	20	6	10	19	10
6	3	109	105	3	13	15	16					1	3	99	91					10	4	15	14	7	9	39	39	8	11	21	20
6	4	60	57	5	0	127	118					1	4	61	66					14	5	48	45	9	1	36	33	8	1	49	48
6	5	66	64	5	1	159	148					1	5	30	30					10	6	15	11	9	3	23	22	8	3	42	42
6	6	7	33	5	2	71	67					1	6	78	81					12	0	15	14	9	4	13	14	8	5	40	40
6	7	11	10	5	3	80	83					1	7	27	27					12	1	31	29	9	5	46	43	8	7	38	38
6	8	33	34	5	4	57	56					1	8	113	112					12	2	32	31	9	6	8	7	8	8	9	5
6	9	40	42	5	5	84	86					1	10	37	36					12	3	9	9	9	8	10	10	8	9	35	33
6	10	10	13	5	6	13	13					1	12	36	36					11	4	10	10	9	9	36	33	10	1	33	30
8	0	9	4	5	7	30	31					1	13	15	13					11	1	50	48	11	1	50	48	10	2	22	20
8	1	47	46	5	8	57	57					3	0	61	60					11	2	33	32	11	2	33	32	10	3	42	39
8	2	8	6	5	9	57	57					3	1	41	40					11	3	27	27	11	3	27	27	10	4	18	19
8	3	55	54	5	10	11	8					3	2	38	39					1	0	90	88	11	4	17	16	10	5	34	33
8	4	21	21	5	11	27	27					3	3	66	61					1	2	295	306	11	5	28	26	10	6	15	13
8	5	70	69	5	12	27	29					3	4	90	91					1	3	84	89					10	7	17	16
8	6	14	15	7	0	38	37					3	5	62	62					1	4	74	79					12	1	22	21
8	7	49	48	7	1	73	73					3	6	59	63					1	5	41	42								
8	8	40	40	7	2	80	76					3	7	29	29					1	6	110	112								
10	0	25	24	7	3	29	29					3	8	65	65					1	8	24	27								
10	1	36	35	7	4	54	52					3	9	36	34					1	9	19	21								
10	2	39	37	7	5	54	52					3	10	29	30					1	10	50	47								
10	3	17	15	7	6	51	51					3	12	37	35					1	12	11	10								
10	4	17	15	7	7	51	51					3	13	21	20					1	13	14	12								
10	5	26	25	7	8	14	12					5	0	7	6					3	0	6	3								
10	6	14	10	7	9	26	27					5	1	121	119					3	1	102	105								
10	7	30	30	7	10	11	12					5	2	138	128					3	2	100	103								
12	0	46	45	7	11	29	28					5	3	56	57					3	3	9	6								
12	1	23	23	9	1	49	46					5	4	67	68					3	4	16	14								
12	2	22	22	9	2	10	13					5	5	95	95					3	5	26	26								
12	3	22	22	9	3	39	37					5	6	38	37					3	6	69	69								
12	4	35	33	9	4	14	13					5	7	17	16					3	7	8	8								
				9	5	38	37					5	8	50	49					3	8	13	15								
				9	6	24	23					5	9	37	36					3	9	56	54								
				9	7	52	48					5	10	17	17					3	10	43	42								
				11	0	42	40					5	12	23	21					3	11	18	14								
				11	1	58	49					7	0	11	13					3	12	20	18								

Table G. (continued)

K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC				
3	6	60	61	4	2	40	43	5	0	43	42	4	8	37	37	7	4	15	13	H= 13	4	4	20	20	2	0	47	48			
3	7	18	19	4	3	82	85	5	1	22	22	4	10	22	23	7	5	17	17		4	5	35	36	2	2	44	46			
3	8	9	10	4	5	6	8	5	2	28	29	4	11	15	15	7	6	10	8	1	3	70	68	4	6	11	12	2	4	27	26
3	9	33	32	4	6	30	41	5	3	82	83	6	0	41	41	7	7	45	46	1	1	35	34	4	7	15	15	2	5	8	8
3	10	42	39	4	7	44	45	5	4	43	42	6	1	14	15	9	0	15	17	1	3	8	7	4	8	18	17	2	6	26	27
3	11	19	17	4	8	18	18	5	5	12	12	6	2	23	22	9	2	10	9	1	4	83	85	6	1	64	70	2	8	29	31
5	0	54	53	4	9	21	19	5	6	35	37	6	3	55	56	9	3	24	23	1	6	9	10	6	2	13	14	4	0	10	11
5	1	85	85	4	10	36	36	5	7	62	62	6	4	30	32	9	5	16	16	1	8	32	33	6	3	11	13	4	1	46	47
5	2	33	35	4	11	18	15	5	8	23	22	6	5	12	12	11	0	19	17	3	0	73	72	6	4	20	21	4	2	46	47
5	3	81	79	6	0	24	24	5	9	8	9	6	6	18	20					3	1	29	30	6	5	28	29	4	3	12	14
5	5	34	35	6	1	22	22	5	11	27	26	6	7	61	60	H= 12				3	2	26	27	6	6	9	11	4	4	10	9
5	6	52	54	6	2	53	51	5	11	13	12	6	8	15	16					3	3	24	24	6	7	14	13	4	5	32	32
5	7	46	46	6	3	77	77	7	0	16	15	6	9	9	7	0	0	90	90	3	4	50	54	6	8	10	12	4	6	11	13
5	8	8	6	6	4	20	18	7	2	22	21	8	1	9	8	0	2	36	37	3	5	24	25	8	1	51	52	4	8	15	15
5	9	31	31	6	5	38	38	7	3	42	41	8	3	40	40	4	4	112	114	3	7	20	22	8	3	14	18	6	0	16	16
5	10	33	32	6	6	10	13	7	4	18	19	8	7	29	29	0	6	13	15	3	8	14	13	8	5	22	22	6	1	45	47
5	11	20	19	6	7	58	59	7	6	9	10	10	0	16	15	0	8	49	47	5	0	31	34					6	2	16	16
7	1	40	39	6	8	22	21	7	7	52	52	10	2	12	9	0	13	8	8	5	1	32	34	H= 15				6	3	11	13
7	2	24	23	6	9	19	20	7	8	11	14	10	3	30	28	2	7	84	84	5	2	12	16					6	4	9	7
7</																															

Table G. (concluded)

K	L	FD	FC
2	6	26	26
4	1	22	22
4	2	29	33
4	3	8	10
4	4	8	7
4	5	16	17
4	6	12	12
6	1	15	16
6	3	23	22

M= 19

1	2	25	24
1	3	9	8
1	6	26	27
3	0	9	8
3	2	31	31
3	3	9	11
3	5	12	11
3	6	14	14
5	1	11	11
5	3	25	28

M= 20

0	2	24	24
0	4	16	16
2	2	28	29
2	4	11	11
4	1	10	7
4	2	13	11
4	3	19	22
4	4	16	15

M= 21

1	0	10	10
1	2	20	20
1	4	13	13
3	2	14	16
3	3	13	13

Table H. Observed (FO) and Calculated (FC) Structure Factors for $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
	H ^a 0			6	11	128	134	12	6	88	92	0	4	19	19	3	15	49	48	6	22	23	22	10	7	18	16	14	10	47	50
0	4	50	37	6	12	160	169	12	7	50	58	0	8	159	169	3	18	27	26	7	1	142	138	10	8	11	11	14	11	13	14
0	6	14	7	6	13	15	21	12	8	40	38	0	10	125	132	3	19	14	12	7	2	83	82	10	10	34	34	14	12	24	23
0	8	175	194	6	14	102	111	12	9	34	34	0	12	106	105	3	20	49	49	7	3	53	93	10	11	45	48	14	13	28	30
0	10	51	53	6	15	46	45	12	10	41	40	0	14	24	25	3	21	30	30	7	4	37	37	10	12	12	11	14	15	14	8
0	12	11	8	6	16	36	37	12	12	17	8	0	16	107	112	3	22	33	29	7	5	69	65	10	13	70	72	14	16	26	29
0	14	53	52	6	17	90	90	12	13	48	55	0	18	76	74	4	1	35	37	7	6	28	28	10	14	17	22	14	18	30	33
0	16	82	84	6	19	12	11	12	14	67	67	0	20	26	25	4	2	29	26	7	7	88	88	10	16	17	14	15	1	93	93
0	18	77	73	6	20	25	26	12	16	21	20	1	1	268	284	4	3	138	130	7	8	20	21	10	17	24	25	15	2	17	17
0	20	45	38	6	21	31	33	12	18	27	28	1	2	191	206	4	4	42	39	7	9	148	149	10	20	19	18	15	3	40	37
0	22	14	10	6	22	19	19	12	19	28	30	1	3	102	110	4	5	216	220	7	10	15	16	10	22	26	25	15	4	18	23
2	0	10	5	8	0	250	245	12	21	43	41	1	4	18	14	4	6	74	72	7	11	43	45	11	2	76	73	15	6	14	11
2	3	49	42	8	1	52	54	14	0	138	132	1	6	27	28	4	7	185	190	7	12	19	23	11	4	137	134	15	7	64	65
2	4	164	170	8	2	196	191	14	1	47	43	1	8	168	174	4	9	9	10	7	13	17	16	11	5	23	20	15	8	19	24
2	5	26	21	8	3	49	51	14	2	82	82	1	9	10	10	4	11	95	105	7	15	28	27	11	6	86	87	15	9	39	41
2	6	105	125	8	4	77	78	14	3	60	59	1	10	94	97	4	12	14	21	7	16	20	20	11	11	15	19	15	17	19	25
2	7	78	90	8	5	9	4	14	4	65	66	1	11	34	32	4	13	128	137	7	17	30	32	11	12	19	21	15	18	17	15
2	8	72	80	8	6	15	17	14	5	22	19	1	12	35	17	4	15	67	70	7	19	49	51	11	14	21	21	15	19	14	12
2	9	198	212	8	7	38	37	14	7	37	41	1	13	60	61	4	17	16	15	7	20	17	18	11	16	20	17	16	1	86	85
2	11	55	124	8	8	92	100	14	8	53	57	1	14	52	54	4	19	34	33	7	23	17	11	11	19	13	15	16	3	32	31
2	12	151	164	8	9	136	149	14	9	49	51	1	15	24	29	4	21	36	36	7	25	24	19	11	20	24	20	16	4	25	21
2	14	140	149	8	10	80	85	14	10	15	18	1	16	85	87	4	23	16	15	8	1	81	76	11	22	29	24	16	5	20	20
2	16	90	89	8	11	67	70	14	11	21	16	1	17	35	40	5	1	102	90	8	2	19	18	12	1	30	28	16	6	23	21
2	17	49	53	8	12	37	40	14	14	23	26	1	18	28	30	5	2	66	59	8	3	8	15	12	2	61	59	16	7	14	12
2	19	49	53	8	14	19	26	14	15	43	44	1	19	33	39	5	3	8	12	8	5	10	8	12	3	64	64	16	9	17	14
2	20	35	31	8	15	16	8	14	16	25	22	1	20	12	8	5	4	92	90	8	6	45	47	12	4	96	97	16	10	17	16
2	22	25	24	8	16	22	16	14	17	22	22	1	23	14	13	5	5	147	151	8	7	37	37	12	5	58	59	16	12	13	16
4	0	63	59	8	20	31	25	16	0	56	55	2	1	203	190	5	6	117	113	8	8	149	154	12	6	48	49	16	13	18	18
4	1	84	92	8	21	15	14	16	1	27	24	2	2	203	197	5	7	71	74	8	10	131	135	12	7	51	52	16	17	16	15
4	2	10	4	10	0	27	28	16	2	36	40	2	3	222	224	5	8	87	93	8	11	20	20	12	8	13	14	17	1	21	19
4	3	259	269	10	1	69	63	16	3	36	36	2	4	148	139	5	10	73	79	8	12	50	51	12	9	12	9	17	5	26	27
4	4	325	329	10	2	54	53	16	4	26	27	2	5	104	104	5	11	70	71	8	14	39	39	12	10	33	33	17	6	17	14
4	5	460	487	10	3	67	64	16	6	28	29	2	7	46	52	5	12	38	37	8	16	45	46	12	11	16	12	17	8	35	38
4	6	169	182	10	4	61	60	16	7	31	28	2	8	23	23	5	13	102	108	8	17	20	23	12	12	15	18	17	10	36	38
4	7	95	98	10	5	109	107	16	8	28	29	2	9	59	60	5	15	56	58	8	18	38	39	12	13	30	28	17	11	16	15
4	8	51	56	10	6	108	109	16	9	84	85	2	10	32	37	5	16	22	23	8	20	25	25	12	14	28	29	17	13	16	16
4	9	49	50	10	7	101	106	16	11	51	53	2	11	30	31	5	17	14	16	9	1	34	33	12	15	35	35	17	16	19	17
4	11	11	13	10	8	72	78	16	15	35	35	2	12	20	22	5	18	42	45	9	3	94	87	12	16	21	19	18	2	17	17
4	12	56	61	10	9	105	109	16	16	15	17	2	14	33	33	5	19	24	21	9	5	44	41	12	20	17	12	18	3	26	26
4	14	29	30	10	10	22	21	16	17	40	40	2	15	14	20	6	1	126	114	9	6	79	82	12	22	23	19	18	5	29	24
4	15	57	60	10	11	50	51	16	18	68	69	2	16	55	56	6	2	72	73	9	7	51	49	13	3	61	61	18	7	18	14
4	16	22	22	10	12	81	84	18	1	34	34	2	17	19	21	6	3	41	42	9	8	118	118	13	5	64	63	18	8	29	31
4	19	25	24	10	13	19	19	18	2	14	11	2	19	42	40	6	4	91	90	9	9	37	30	13	6	13	12	18	10	25	23
4	21	56	54	10	14	16	20	18	3	88	89	2	20	35	31	6	6	122	121	9	10	140	149	13	7	24	22	18	11	17	16
4	23	57	56	10	16	17	23	18	4	26	26	2	22	36	34	6	7	94	97	9	11	45	46	13	8	48	49	18	13	32	33
6	0	208	189	10	17	29	27	18	5	58	59	3	1	22	15	6	8	92	91	9	13	36	38	13	11	20	18	19	2	48	49
6	1	30	22	10	19	29	30	18	6	24	21	3	2	63	62	6	9	21	20	9	14	49	51	13	13	68	68	19	4	45	46
6	2	184	182	10	20	24	20	18	7	25	22	3	3	142	143	6	10	19	21	9	15	17	18	13	15	55	56	19	5	22	19
6	3	113	117	10	21	23	22	18	8	18	17	3	4	533	524	6	11	57	58	9	16	28	28	13	16	18	20	19	6	19	19
6	4	160	161	10	23	17	19	18	9	21	20	3	5	183	183	6	12	15	15	9	20	19	20	14	1	46	47	19	11	16	17
6	5	49	45	12	0	37	37	18	12	19	21	3	6	177	176	6	13	25	28	10	1	120	113	14	2	14	12	20	1	16	12
6	6	153	162	12	1	58	57	18				3	7	123	128	6	14	18	22	10	2	27	27	14	4	26	26	20	2	31	28
6	7	75	79	12	2	39	37		H ^a 1			3	8	21	27	6	17	35	36	10	3	74	71	14	5	45	44	20	4	40	38
6	8	73	79	12	3	83	80					3	9	34	35	6	18	13	15	10	4	93	93	14	6	40	40	20	6	27	27
6	9	76	83	12																											

Table H. (continued)

K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC	K	L	FC	FC
H= 2				3	3	153	161	6	5	106	99	9	10	29	32	14	3	23	23	0	20	43	41	3	19	36	34	6	20	35	33	3	19	36	34
0	0	159	122	3	4	194	185	6	6	115	105	9	12	13	16	14	6	24	29	0	22	21	21	3	20	43	44	6	22	20	20	3	20	43	44
0	4	46	44	3	5	151	145	6	7	54	57	9	15	18	20	14	7	15	14	0	24	14	15	3	22	33	36	6	23	15	8	3	22	33	36
0	6	65	65	3	6	67	69	6	8	145	148	9	16	35	36	14	10	30	31	1	1	197	173	3	24	17	20	7	1	193	194	7	2	29	29
0	8	14	17	3	7	50	50	6	9	44	53	9	18	53	54	14	12	12	12	4	1	16	9	4	1	16	9	7	3	68	69	7	3	68	69
0	10	34	34	3	9	64	60	6	10	11	19	9	19	16	16	15	0	38	37	1	5	58	52	4	3	85	84	7	4	74	76	7	4	74	76
0	12	26	23	3	10	61	63	6	11	50	48	9	20	45	44	15	1	26	24	1	6	41	41	4	4	44	41	7	6	60	58	7	6	60	58
0	14	10	11	3	12	149	155	6	12	18	19	9	21	28	23	15	2	33	33	1	7	53	52	4	5	153	150	7	7	95	98	7	7	95	98
1	0	212	193	3	13	34	39	6	13	12	10	9	23	23	24	15	3	43	42	1	8	64	64	4	6	68	64	7	9	129	128	7	9	129	128
1	1	98	90	3	14	140	141	6	14	15	14	9	24	24	19	15	4	25	25	1	9	79	77	4	7	111	111	7	10	55	53	7	10	55	53
1	2	11	14	3	15	57	60	6	21	15	17	10	0	45	43	15	5	14	15	1	10	107	112	4	8	84	83	7	14	32	32	7	14	32	32
1	3	10	11	3	16	72	70	6	22	14	16	10	1	62	50	15	7	55	54	1	11	9	15	4	9	71	65	7	15	19	21	7	15	19	21
1	4	99	91	3	17	46	49	7	0	100	96	10	2	36	37	15	9	74	75	1	12	65	69	4	10	38	28	7	16	22	20	7	16	22	20
1	5	108	111	3	21	24	21	7	2	44	45	10	5	33	34	15	11	67	66	1	13	64	65	4	11	110	109	7	17	31	38	7	17	31	38
1	6	52	54	3	22	24	21	7	3	65	62	10	7	15	11	15	15	25	26	1	14	18	18	4	12	16	15	7	19	36	32	7	19	36	32
1	7	142	152	4	0	8	10	7	4	16	18	10	9	16	18	15	17	41	40	1	15	75	75	4	13	106	109	7	21	28	26	7	21	28	26
1	8	76	80	4	1	9	12	7	5	61	58	10	11	19	18	16	3	13	16	1	16	35	31	4	15	91	93	7	22	24	24	7	22	24	24
1	9	144	151	4	2	29	25	7	6	45	48	11	0	28	29	16	6	28	26	1	17	42	38	4	17	20	18	7	24	18	18	7	24	18	18
1	10	44	43	4	3	72	62	7	7	171	175	11	1	31	28	16	8	22	24	1	18	31	28	4	18	25	24	8	1	128	123	8	1	128	123
1	11	86	92	4	4	8	2	7	8	97	95	11	2	18	21	16	11	19	17	1	25	14	7	4	23	14	18	8	2	53	51	8	2	53	51
1	12	58	61	4	5	55	53	7	9	232	242	11	3	13	13	17	0	88	78	2	1	160	162	5	1	93	97	8	3	32	28	8	3	32	28
1	13	25	26	4	6	31	27	7	11	143	147	11	4	94	94	17	1	26	21	2	2	66	54	5	2	34	29	8	4	27	28	8	4	27	28
1	14	41	42	4	7	77	76	7	12	35	37	11	5	11	7	17	2	63	63	2	3	16	32	5	3	11	11	8	5	33	35	8	5	33	35
1	15	27	29	4	8	62	62	7	13	17	21	11	6	123	123	17	3	44	40	2	4	127	123	5	4	29	31	8	6	31	35	8	6	31	35
1	16	31	28	4	12	16	18	7	14	24	23	11	7	25	27	17	4	25	25	2	5	38	38	5	5	150	145	8	7	37	35	8	7	37	35
1	17	67	70	4	13	14	14	7	15	65	64	11	8	55	54	17	5	25	24	2	6	107	103	5	6	42	42	8	8	104	107	8	8	104	107
1	18	61	60	4	16	11	5	7	16	23	30	11	9	43	43	17	8	29	28	2	7	40	40	5	7	154	151	8	9	37	36	8	9	37	36
1	19	64	64	4	17	14	18	7	17	86	89	11	10	68	70	17	9	23	22	2	8	63	62	5	8	17	13	8	10	125	124	8	10	125	124
1	20	48	47	4	20	12	11	7	18	25	31	11	12	145	151	17	10	32	34	2	9	59	57	5	9	59	64	8	12	78	67	8	12	78	67
1	21	44	42	5	0	147	143	7	19	40	44	11	14	120	125	17	11	15	15	2	10	17	17	5	11	86	84	8	15	12	13	8	15	12	13
1	23	25	27	5	1	75	81	7	20	20	21	11	16	59	59	17	12	15	19	2	11	14	17	5	12	42	43	8	16	64	66	8	16	64	66
1	24	21	13	5	2	46	49	7	21	14	18	11	17	22	22	17	14	19	18	2	13	52	52	5	13	92	89	8	18	49	49	8	18	49	49
1	26	23	18	5	3	205	207	7	24	16	17	11	20	21	20	17	15	23	18	2	14	26	26	5	15	51	50	8	19	19	19	8	19	19	19
2	0	18	16	5	4	89	88	8	0	21	22	11	22	19	16	18	1	13	17	2	15	71	72	5	16	29	27	8	20	21	21	8	20	21	21
2	1	21	19	5	5	218	215	8	2	15	18	12	0	18	16	19	1	15	11	2	16	18	18	5	18	39	36	9	1	48	46	9	1	48	46
2	2	31	32	5	7	11	5	8	3	12	13	12	2	29	31	19	3	16	15	2	17	39	40	5	19	16	16	9	2	117	113	9	2	117	113
2	3	100	101	5	8	50	49	8	4	51	47	12	3	24	24	19	4	16	14	2	19	36	35	5	20	21	16	9	4	67	69	9	4	67	69
2	4	28	25	5	9	63	66	8	5	10	12	12	4	14	16	19	5	20	16	2	20	31	27	5	22	15	14	9	5	43	46	9	5	43	46
2	5	51	42	5	10	37	39	8	6	20	17	12	8	20	24	19	6	29	29	2	21	13	12	6	1	89	81	9	7	30	31	9	7	30	31
2	6	10	5	5	11	12	15	8	7	22	24	12	11	24	24	19	7	18	14	2	22	32	31	6	2	99	99	9	8	96	99	9	8	96	99
2	7	14	11	5	12	90	94	8	8	16	16	12	12	12	12	19	10	19	22	2	24	23	18	6	3	10	8	9	10	102	104	9	10	102	104
2	8	40	39	5	14	68	67	8	10	14	12	13	0	107	103	21	0	21	19	3	1	10	10	6	4	117	113	9	11	62	63	9	11	62	63
2	9	26	25	5	15	46	46	8	12	22	31	13	1	55	52	21	3	22	19	3	2	187	185	6	5	93	87	9	12	47	49	9	12	47	49
2	10	76	73	5	16	54	52	8	13	24	30	13	2	75	74					3	4	153	155	6	6	48	51	9	13	57	61	9	13	57	61
2	11	81	81	5	17	19	16	8	14	21	29	13	3	129	126					3	5	52	55	6	7	59	55	9	14	48	43	9	14	48	43
2	12	69	74	5	18	27	29	9	0	215	203	13	5	110	108					3	6	87	93	6	8	75	73	9	15	16	15	9	15	16	15
2	13	12	16	5	19	23	23	9	1	32	29	13	6	38	36	0	2	18	11	3	7	37	40	6	9	59	59	9	16	54	54	9	16	54	54
2	14	18	19	5	21	44	42	9	2	112	109	13	7	29	28	0	4	21	20	3	8	113	119	6	10	71	71	9	18	35	37	9	18	35	37
2	15	11	10	5	23	41	37	9	3	65	62	13	8	28	23	0	6	40	37	3	9	36	35	6	12	18	13	10	1	66	64	10	1		

Table H. (continued)

K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC
10	9	29	27	14	8	46	47	0	20	36	36	4	4	39	39	7	5	55	52	10	21	23	21	15	12	14	17	2	3	74	71
10	10	47	49	14	10	41	42	0	24	39	33	4	5	269	260	7	6	17	16	11	0	23	22	16	0	41	41	2	4	128	125
10	11	38	38	14	11	22	24	1	0	36	32	4	6	58	57	7	9	29	30	11	1	26	22	16	1	16	19	2	5	59	60
10	12	15	13	14	12	17	15	1	1	105	94	4	7	70	72	7	10	16	13	11	2	27	29	16	2	26	25	2	6	33	36
10	13	61	64	14	13	16	20	1	2	40	34	4	8	26	29	7	11	26	26	11	5	24	23	16	7	30	28	2	7	89	89
10	15	62	67	14	16	16	18	1	3	88	73	4	10	41	38	7	12	13	16	11	9	17	20	16	8	16	15	2	8	44	43
10	16	25	25	14	18	29	27	1	4	45	80	4	12	43	43	7	13	29	28	11	10	20	24	16	9	62	64	2	9	60	61
10	17	28	28	15	1	79	80	1	5	12	7	4	13	12	12	7	14	25	31	11	12	20	22	16	10	19	17	2	10	71	72
10	19	13	11	15	2	15	11	1	6	70	72	4	14	32	32	7	15	26	31	11	13	18	17	16	11	46	45	2	11	24	23
10	20	24	22	15	3	21	19	1	7	19	22	4	15	31	28	7	16	13	11	11	15	13	5	16	15	24	25	2	12	31	30
11	22	23	25	15	5	38	39	1	9	36	36	4	16	13	13	7	17	18	19	11	17	23	24	17	0	17	19	2	14	24	26
11	1	56	56	15	6	12	18	1	10	19	16	4	19	46	46	7	18	16	17	12	0	37	38	17	3	13	13	2	15	15	19
11	2	76	74	15	7	38	40	1	11	34	35	4	21	53	43	8	0	241	237	12	1	14	15	17	6	22	22	2	16	41	41
11	4	125	122	15	8	13	14	1	12	21	19	4	23	41	34	8	1	30	25	12	3	80	81	17	13	14	6	2	17	20	21
11	5	23	25	15	9	37	38	1	13	18	19	5	0	65	50	2	0	133	135	12	4	57	58	18	0	22	19	2	19	26	23
11	6	66	65	15	17	21	19	1	14	17	21	5	1	16	12	8	3	67	64	12	5	100	99	18	1	20	24	2	20	15	14
11	7	26	27	16	1	59	59	1	15	16	18	5	2	39	34	0	5	10	11	12	6	75	74	18	2	14	12	2	22	32	20
11	10	41	47	16	3	29	26	1	23	16	13	5	3	70	67	8	6	53	52	12	7	51	52	18	3	51	50	2	24	20	16
11	11	20	24	16	4	13	5	2	0	12	17	5	4	41	37	8	7	49	49	12	8	31	35	18	5	47	45	3	1	82	76
11	12	16	18	16	5	15	18	2	1	59	55	5	5	9	2	8	8	79	78	12	9	11	14	18	6	27	26	3	2	65	66
11	14	16	12	16	7	25	25	2	2	8	12	5	6	97	95	8	9	84	83	12	10	17	14	18	7	24	27	3	3	39	40
11	16	26	30	16	8	22	22	2	3	25	17	5	7	36	33	8	10	45	46	12	12	55	56	19	1	17	16	3	4	100	103
11	20	23	20	16	9	18	17	2	4	37	37	5	8	25	21	8	11	56	55	12	14	56	56	20	4	18	17	3	5	53	56
11	22	27	26	16	10	28	28	2	5	46	76	5	9	39	40	8	13	12	17	12	10	21	22	3	8	120	119	3	6	120	119
12	1	20	22	16	12	20	17	2	6	112	114	5	10	26	26	8	15	30	24	12	20	17	14								
12	2	49	50	17	1	26	25	2	7	108	110	5	11	45	47	8	16	32	31	13	0	32	30								
12	3	22	22	17	3	18	19	2	8	71	71	5	13	16	18	8	17	23	19	13	1	24	28	0	2	35	36	3	9	14	14
12	4	82	82	17	5	18	21	2	9	156	155	5	14	35	35	8	18	51	48	13	2	13	11	0	4	85	79	3	10	30	28
12	5	61	64	17	7	14	13	2	10	49	49	5	18	15	15	8	19	19	17	13	3	12	13	0	6	81	79	3	11	53	52
12	6	39	42	17	8	20	19	2	11	87	89	5	19	22	22	8	20	28	29	13	5	13	12	0	8	124	124	3	12	21	20
12	7	48	48	17	9	16	18	2	12	129	129	5	20	18	14	9	0	19	19	13	6	16	18	0	10	160	169	3	13	71	72
12	11	32	32	17	10	24	22	2	13	22	25	6	0	39	41	9	5	20	23	13	8	24	24	0	12	43	42	3	14	27	30
12	12	14	13	17	12	16	18	2	14	101	97	6	1	19	19	9	6	25	27	13	9	14	18	0	14	66	67	3	15	39	41
12	13	53	53	17	13	24	24	2	15	31	33	6	2	74	76	9	7	20	18	13	10	13	17	0	16	28	26	3	16	18	19
12	15	35	36	18	15	15	16	2	16	37	36	6	3	96	96	9	11	29	32	14	0	62	61	8	18	35	38	3	17	14	13
12	16	17	18	18	11	30	31	2	17	61	57	6	4	120	119	9	14	24	26	14	1	21	23	0	22	17	15	3	18	25	27
12	17	15	13	18	13	27	27	2	19	29	24	6	5	52	51	9	19	24	26	14	2	63	61	0	24	25	21	3	19	18	14
12	20	15	16	19	2	20	21	2	20	17	16	6	6	63	63	10	0	133	131	14	3	57	57	1	1	218	202	3	20	25	23
13	2	38	36	19	4	34	33	3	0	175	157	6	7	85	86	10	1	21	22	14	4	24	22	1	2	17	17	3	22	24	26
13	4	46	46	19	6	17	17	3	1	20	17	6	8	16	15	10	2	54	56	14	5	44	44	1	3	93	94	4	1	12	18
13	5	42	41	20	2	19	21	3	2	181	92	6	9	105	112	10	3	60	69	14	6	19	23	1	4	72	66	4	2	39	40
13	7	43	43	20	4	28	29	3	3	14	18	6	10	65	63	18	4	49	48	14	7	20	22	1	5	65	64	4	3	73	69
13	8	50	50	20	6	18	22	3	4	26	22	6	11	41	80	10	5	97	97	14	8	31	32	1	7	16	14	4	4	18	18
13	9	30	32					3	5	37	33	6	12	108	112	10	6	87	85	14	9	52	56	1	8	110	110	4	5	107	108
13	10	43	41					3	6	63	55	6	14	89	89	10	7	82	83	14	10	27	26	1	9	47	44	4	6	31	31
13	11	41	42					3	7	42	38	6	15	53	54	10	8	50	49	14	11	23	26	1	10	100	101	4	7	46	47
13	13	50	53	0	0	309	308	3	8	25	23	6	16	47	49	10	9	71	71	14	12	23	20	1	11	44	44	4	8	39	37
13	15	43	46	0	2	282	276	3	9	18	19	6	17	65	64	10	10	20	19	14	14	28	25	1	12	16	21	4	9	16	17
13	16	17	12	0	4	64	64	3	10	27	26	6	18	20	28	10	11	38	38	14	15	26	24	1	13	27	20	4	10	32	32
13	19	17	15	0	6	122	126	3	11	26	27	6	19	29	30	10	12	58	57	14	16	19	20	1	14	19	16	4	11	76	76
14	1	33	34	0	8	133	135	3	12	17	17	6	21	15	16	10	13	15	17	14	17	18	14	1	15	17	15	4	13	108	106
14	3	15	14	0	10	51	49	3	14	11	13	6	23	15	12	10	14	56	54	14	18	16	17	1	16	34	32	4	14	23	22
14	4	13	14	0	12	15	16	3	18	23	23	7	0	27	26	10	17	13	21	15	0	38	39	1	18	25	25	4	15	71	71
14	5	45	47	0	14	63	67	4	0	19	17	7	2	42	42	10	18	11	34	15	2	22	23	1	19	16	14	4	16	37	37
14	6	61	61	0	16	72	73	4	1	82	79	7	3	41	40	10	19	33	33	15	6	18	15	2	1	101	103	4	19	40	39
14	7	38	34	0	18	54	55	4	3	266	257	7	4	15	16	10	20	21	20	15	9	14	13</								

Table H. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
5	1	17	14	8	4	32	26	12	11	41	40	19	4	33	33	3	14	87	89	7	14	22	20	13	13	17	21	2	12	20	18	2	12	20	18
5	2	70	73	8	5	44	42	12	13	37	34					3	15	25	26	7	15	47	50	14	6	17	19	2	13	22	23	2	13	22	23
5	3	50	53	8	6	57	54	12	14	18	20		H*	6		3	16	21	23	7	17	59	57	14	9	15	11	2	15	54	51	2	15	54	51
5	4	96	94	8	7	16	15	12	15	16	13					3	17	48	50	7	19	47	42	14	10	15	14	2	16	24	21	2	16	24	21
5	5	77	74	8	8	91	88	13	1	54	53	0	0	53	49	3	21	38	35	8	0	15	22	14	14	19	13	2	17	23	23	2	17	23	23
5	6	77	78	8	10	60	59	13	2	13	14	0	2	12	11	3	22	14	14	8	1	13	12	15	1	13	12	2	19	25	23	2	19	25	23
5	7	19	23	8	12	21	20	13	3	29	31	0	4	36	35	4	0	11	6	8	2	33	31	15	3	24	21	2	20	31	27	2	20	31	27
5	8	51	48	8	13	15	16	13	5	51	54	0	6	33	30	4	1	17	16	8	3	40	36	15	4	14	16	3	1	49	46	3	1	49	46
5	10	27	29	8	14	26	27	13	6	26	24	0	8	32	29	4	5	14	10	8	4	18	13	15	6	15	11	3	2	51	49	3	2	51	49
5	11	46	44	8	16	41	41	13	7	29	29	0	10	37	34	4	6	15	14	8	7	14	14	15	7	45	47	3	4	98	88	3	4	98	88
5	13	71	68	8	17	17	13	13	8	29	26	0	12	32	33	4	7	28	30	8	9	13	14	15	8	14	11	3	5	89	88	3	5	89	88
5	15	44	44	8	18	17	20	13	10	27	27	0	14	20	20	4	8	11	1	8	11	18	12	15	9	53	55	3	6	100	96	3	6	100	96
5	16	13	13	8	19	26	24	13	11	42	42	0	20	14	9	4	9	39	38	8	12	17	19	15	11	42	42	3	7	102	102	3	7	102	102
5	18	19	12	8	20	15	17	13	13	34	34	1	8	130	136	4	10	24	22	8	14	20	20	16	3	15	17	3	8	28	25	3	8	28	25
5	19	14	15	9	1	75	76	13	14	15	14	1	2	140	143	4	13	14	11	9	0	225	218	17	0	62	60	3	9	19	17	3	9	19	17
5	20	18	18	9	2	24	21	13	15	21	21	1	3	38	37	5	0	101	98	9	1	22	21	17	1	15	16	3	11	30	29	3	11	30	29
5	21	15	13	9	3	74	76	13	16	17	16	1	4	20	13	5	1	74	76	9	2	95	92	17	2	50	50	3	12	14	14	3	12	14	14
5	22	16	19	9	5	35	35	14	1	37	36	1	5	72	71	9	2	107	103	9	3	74	75	17	3	31	29	3	13	27	20	3	13	27	20
6	1	115	115	9	6	61	60	14	2	25	23	1	6	132	132	3	5	156	157	9	5	43	43	17	5	31	29	3	14	13	11	3	14	13	11
6	2	33	32	9	8	73	73	14	4	34	32	1	7	131	133	5	4	122	116	9	7	16	20	17	6	15	7	3	15	21	19	3	15	21	19
6	3	69	66	9	9	12	9	14	5	28	30	1	8	114	114	5	5	141	139	9	8	20	18	17	8	17	19	3	17	14	11	3	17	14	11
6	4	55	57	9	10	61	61	14	6	48	48	1	9	147	143	5	6	146	146	9	9	22	20	17	9	29	31	3	18	16	14	3	18	16	14
6	5	19	22	9	11	20	20	14	7	41	42	1	11	75	71	5	7	135	131	9	11	16	18	17	10	16	18	3	19	24	22	3	19	24	22
6	6	39	39	9	12	25	25	14	8	46	47	1	12	88	91	5	8	130	128	9	16	18	19	17	11	18	19	3	20	20	20	3	20	20	20
6	7	93	96	9	13	23	20	14	9	19	21	1	13	15	12	5	9	49	46	9	10	34	33	17	12	14	12	4	1	40	38	4	1	40	38
6	8	28	30	9	15	18	19	14	10	30	29	1	14	16	16	5	10	15	13	9	20	14	12	0	6	93	95	4	2	54	55	4	2	54	55
6	9	13	10	9	16	35	34	14	11	20	20	1	15	28	30	5	11	17	16	10	0	56	58	0	8	128	129	4	3	69	68	4	3	69	68
6	10	12	10	9	18	20	19	14	12	18	20	1	17	27	25	5	12	23	25	10	1	18	19	0	10	134	136	4	4	66	69	4	4	66	69
6	11	35	34	10	1	66	66	14	13	28	27	1	18	27	25	5	13	17	14	10	2	31	28	0	14	29	28	4	5	89	83	4	5	89	83
6	11	43	44	10	2	55	94	14	16	19	16	1	19	31	29	5	14	39	39	10	3	26	22	0	18	25	28	4	6	34	35	4	6	34	35
6	15	18	22	10	3	68	68	15	1	58	58	1	20	38	37	5	15	37	37	10	4	16	13	0	20	18	19	4	8	26	22	4	8	26	22
6	16	22	24	10	4	64	64	15	3	38	40	1	21	20	21	5	16	33	32	10	5	34	31	1	1	54	57	4	9	23	26	4	9	23	26
6	17	22	23	10	5	32	30	15	7	32	33	2	0	20	23	5	17	15	13	10	8	23	20	1	2	51	53	4	11	52	53	4	11	52	53
6	18	17	15	10	6	38	38	15	9	22	22	2	1	22	23	5	18	13	12	10	11	14	14	1	3	32	33	4	13	77	74	4	13	77	74
6	19	30	28	10	10	12	14	15	10	15	18	2	2	15	17	5	19	18	17	11	0	54	50	1	4	57	59	4	14	27	23	4	14	27	23
6	21	29	29	10	11	34	36	16	1	41	40	2	3	61	59	5	21	27	26	11	2	48	47	1	7	25	27	4	15	56	55	4	15	56	55
7	1	177	176	10	12	13	10	16	2	15	11	2	5	68	64	6	1	26	28	11	3	12	10	1	8	61	63	4	16	13	11	4	16	13	11
7	2	59	59	10	13	35	33	16	5	26	26	2	6	24	21	6	3	52	49	11	4	57	61	1	9	13	11	5	1	58	59	5	1	58	59
7	3	88	79	10	14	16	13	16	6	25	25	2	7	21	14	6	4	34	33	11	6	57	57	1	10	96	98	5	2	38	38	5	2	38	38
7	4	29	27	10	16	35	36	16	7	32	32	2	8	42	43	6	5	29	28	11	7	14	16	1	11	17	15	5	3	14	11	5	3	14	11
7	5	22	22	11	2	83	77	16	9	21	20	2	9	20	20	6	6	26	27	11	8	13	9	1	12	44	42	5	4	18	18	5	4	18	18
7	7	26	20	11	3	31	35	16	13	14	11	2	10	34	34	6	7	11	15	11	9	26	24	1	14	24	24	5	5	89	90	5	5	89	90
7	8	26	25	11	4	75	75	17	4	15	10	2	13	22	20	6	8	24	24	11	10	34	32	1	16	37	35	5	6	22	19	5	6	22	19
7	3	46	42	11	5	19	22	17	5	18	20	3	0	30	34	6	10	24	20	11	12	71	69	1	17	30	26	5	7	82	79	5	7	82	79
7	10	21	20	11	6	56	57	17	6	26	26	3	1	42	44	6	18	15	16	11	14	63	61	1	18	24	23	5	8	20	24	5	8	20	24
7	11	24	27	11	8	34	35	17	7	20	22	3	2	83	86	7	0	63	56	11	16	20	23	1	19	17	14	5	9	29	28	5	9	29	28
7	12	16	12	11	10	21	22	17	8	31	32	3	3	115	118	7	1	16	13	12	2	29	28	2	1	69	65	5	10	20	19	5	10	20	19
7	13	15	10	11	12	24	23	17	10	32	30	3	4	76	79	7	2	38	35	12	4	13	12	2	3	33	31	5	13	38	41	5	13	38	41
7	15	39	40	12	1	13	14	18	2	16	15	3	5	45	45	7	3	35	34	12	7	17	21	2	4	76	76	5	15	27	27	5	15	27	27
7	16	22	20	12	2	31	31	18	3	22	23	3</																							

Table H. (concluded)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
6	5	20	20	11	4	57	55	2	1	15	16	6	12	46	45	12	12	41	40	4	9	22	20	11	2	20	20	6	5	23	20	6	5	23	20
6	6	60	60	11	6	31	31	2	2	12	13	6	14	55	52	13	0	16	14	4	10	26	26	11	4	45	42	6	6	31	33	6	6	31	33
6	7	65	66	11	16	16	17	2	4	31	36	6	15	34	35	14	0	39	35	4	11	61	59	11	6	40	41	7	0	26	26	7	0	26	26
6	9	25	24	12	1	16	18	2	6	65	67	6	16	27	29	14	1	23	24	4	13	40	49	11	8	22	24	7	2	21	20	7	2	21	20
6	10	47	46	12	4	44	43	2	7	66	69	6	17	39	38	14	2	25	27	4	15	33	32	12	2	36	34	7	5	29	29	7	5	29	29
6	12	24	31	12	6	27	26	2	8	35	36	7	0	64	62	14	3	37	36	5	3	23	25	12	4	31	31	7	6	23	20	7	6	23	20
6	16	19	19	12	7	22	19	2	9	69	73	7	2	21	21	14	5	16	22	5	4	39	32	12	6	21	17	7	7	36	39	7	7	36	39
6	17	19	20	12	8	16	15	2	10	37	39	7	3	34	36	14	8	19	18	5	5	38	37	12	6	21	17	7	8	20	21	7	8	20	21
6	18	32	31	12	11	34	38	2	11	41	38	7	4	22	23	15	5	19	22	5	6	58	58	13	3	29	26	7	9	47	52	7	9	47	52
6	20	25	23	12	13	35	35	2	12	66	68	7	11	14	12					5	7	17	17					8	2	16	16	8	2	16	16
7	1	99	102	12	15	23	24	2	13	15	19	7	12	15	7					5	8	15	17					8	3	21	20	8	3	21	20
7	2	61	59	13	1	14	12	2	14	58	58	8	0	89	91					5	10	17	18					8	4	32	31	8	4	32	31
7	3	63	64	13	2	31	30	2	15	24	21	8	1	17	15					5	11	36	34					8	5	17	17	8	5	17	17
7	4	52	50	13	3	21	16	2	17	24	23	8	2	79	85					5	13	31	35					8	6	24	25	8	6	24	25
7	5	23	20	13	4	35	37	2	19	19	15	8	3	36	34					5	15	15	18					9	0	67	66	9	0	67	66
7	6	15	7	13	5	32	27	3	2	20	20	8	5	26	23					6	1	53	54					9	1	16	14	9	1	16	14
7	7	17	19	13	7	30	28	3	3	13	10	8	6	40	41					6	2	46	45					9	2	56	56	9	2	56	56
7	10	20	22	13	8	22	22	3	4	16	20	8	7	22	22					6	4	28	26					9	3	32	33	9	3	32	33
7	12	20	22	13	10	24	25	3	5	27	29	8	8	42	40					6	5	41	44					9	5	27	27	9	5	27	27
7	16	21	22	13	11	30	30	3	6	26	26	8	9	38	41					6	6	16	13					9	6	34	34	9	6	34	34
7	17	19	21	13	13	28	28	3	9	41	40	8	10	31	30					6	7	40	40					10	0	18	17	10	0	18	17
7	19	24	18	14	1	28	27	3	14	30	31	8	11	24	21					6	9	21	21					10	2	16	13	10	2	16	13
8	1	87	84	14	4	36	37	3	16	16	19	8	15	21	21					6	10	20	20												
8	3	21	17	14	5	30	31	3	17	14	10	9	16	26	26					7	1	58	64												
8	4	35	37	14	6	39	41	4	1	43	45	9	0	15	15					7	3	43	49												
8	6	35	33	14	7	19	18	4	2	16	19	9	1	16	17					7	4	22	22												
8	7	16	18	14	8	24	23	4	3	106	108	9	5	15	18					7	5	16	17												
8	8	43	45	14	10	22	21	4	5	72	76	9	6	24	27					7	6	22	22												
8	10	43	45	15	1	51	50	4	7	44	47	9	8	16	10					7	7	13	11												
8	12	16	16	15	3	27	25	4	12	35	34	9	12	15	24					7	10	21	22												
8	16	27	29	15	7	27	30	4	13	34	31	9	14	23	21					7	12	16	12												
8	18	27	26	16	1	22	24	4	14	22	22	9	15	16	13					7	13	18	20												
9	2	34	36	16	6	24	26	4	16	14	16	10	0	55	58					8	1	35	40												
9	4	16	19	17	1	22	18	5	0	45	46	10	1	15	19					8	2	16	16												
9	5	23	23					5	2	13	13	10	2	39	37					8	4	14	14												
9	8	41	41					5	3	13	16	10	3	25	28					8	5	29	29												
9	10	55	54					5	5	15	11	10	5	25	30					8	6	25	27												
9	11	14	14					5	6	14	15	10	6	51	50					8	7	37	36												
9	12	20	23					5	7	23	23	10	7	52	53					8	8	39	36												
9	13	29	30					5	9	23	21	10	8	35	36					8	9	16	18												
9	14	16	18					5	10	14	12	10	9	40	39					8	10	48	45												
9	15	24	22					5	11	28	28	10	11	21	19					8	12	19	19												
9	16	40	36					5	13	15	12	10	12	39	41					8	13	18	15												
9	18	22	21					5	16	16	13	10	14	40	41					9	1	28	29												
10	1	73	73					5	17	20	19	11	0	30	32					9	6	24	22												
10	2	62	61					6	0	50	49	11	1	19	19					9	8	41	40												
10	4	41	41					6	1	47	44	11	4	23	17					9	10	43	41												
10	5	21	18					6	2	67	64	11	6	23	19					9	11	27	23												
10	7	15	11					6	3	63	63	12	0	33	34					10	1	18	13												
10	10	14	10					6	4	42	42	12	1	23	23					10	2	49	52												
10	11	30	34					6	5	14	13	12	3	57	57					10	4	61	68												
10	13	33	32					6	6	18	19	12	4	28	28					10	6	15	17												
10	15	28	26					6	7	35	42	12	5	47	48					10	8	28	28												
10	17	21	23					6	9	72	71	12	6	36	37					10	9	16	13												
11	2	53	57					6	10	32	29	12	7	26	25					10	10	36	37												
11	1	20	19					6	11	48	51	12	10	20	23					11	1	21	24												

Table I. Observed (FO) and Calculated (FC) Structure Factors for $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
H=-21				H=-18				H=-16				H=-14				H=-12				H=-10				H=-8				H=-6			
0	2	70	75	4	1	15	13	0	2	33	33	9	7	38	39	0	2	14	12	0	2	30	30	0	2	14	12	0	2	14	12
1	2	22	19	5	2	15	19	10	1	25	25	4	6	32	31	1	1	59	63	1	1	59	63	1	1	59	63	1	1	59	63
3	1	23	26	6	4	21	18	0	6	43	44	5	1	13	16	0	6	34	29	0	6	34	29	0	6	34	29	0	6	34	29
3	2	19	23	8	3	23	19	1	3	49	46	5	2	77	77	1	3	41	48	1	3	41	48	1	3	41	48	1	3	41	48
4	1	49	57	9	2	17	16	1	4	35	30	10	5	53	54	2	4	19	14	2	4	19	14	2	4	19	14	2	4	19	14
4	2	22	27					1	5	33	31	11	1	17	17	3	5	19	19	3	5	19	19	3	5	19	19	3	5	19	19
								1	7	62	60	11	2	38	38	4	6	26	26	4	6	26	26	4	6	26	26	4	6	26	26
								2	2	32	33	11	3	14	13	5	7	38	38	5	7	38	38	5	7	38	38	5	7	38	38
								2	3	57	59	12	1	17	20	6	8	49	52	6	8	49	52	6	8	49	52	6	8	49	52
								2	4	27	25	12	4	29	32	7	9	57	59	7	9	57	59	7	9	57	59	7	9	57	59
								2	5	65	67	12	5	22	22	7	10	67	67	7	10	67	67	7	10	67	67	7	10	67	67
								2	6	41	39	12	6	18	22	7	11	67	63	7	11	67	63	7	11	67	63	7	11	67	63
								3	8	34	30	13	1	21	22	7	12	62	60	7	12	62	60	7	12	62	60	7	12	62	60
								3	1	38	41	13	4	31	28	7	13	62	63	7	13	62	63	7	13	62	63	7	13	62	63
								3	2	33	35	13	5	18	16	7	14	62	63	7	14	62	63	7	14	62	63	7	14	62	63
								3	4	52	52	14	2	22	20	7	15	62	63	7	15	62	63	7	15	62	63	7	15	62	63
								3	5	42	44	14	3	35	40	8	1	50	49	8	1	50	49	8	1	50	49	8	1	50	49
								3	6	29	30	15	1	31	27	8	2	16	16	8	2	16	16	8	2	16	16	8	2	16	16
								3	7	42	43	16	1	28	26	8	3	91	89	8	3	91	89	8	3	91	89	8	3	91	89
								4	1	26	26					8	4	18	17	8	4	18	17	8	4	18	17	8	4	18	17
								4	2	15	10					8	5	26	25	8	5	26	25	8	5	26	25	8	5	26	25
								4	3	27	25					8	6	44	44	8	6	44	44	8	6	44	44	8	6	44	44
								4	4	49	48					8	7	40	39	8	7	40	39	8	7	40	39	8	7	40	39
								4	5	17	16					8	8	25	24	8	8	25	24	8	8	25	24	8	8	25	24
								4	6	17	18					9	2	34	31	9	2	34	31	9	2	34	31	9	2	34	31
								4	7	27	27					9	3	49	47	9	3	49	47	9	3	49	47	9	3	49	47
								5	1	14	12					9	4	38	37	9	4	38	37	9	4	38	37	9	4	38	37
								5	2	30	26					9	5	35	32	9	5	35	32	9	5	35	32	9	5	35	32
								5	3	36	33					10	1	27	28	10	1	27	28	10	1	27	28	10	1	27	28
								5	4	65	66					10	2	26	21	10	2	26	21	10	2	26	21	10	2	26	21
								5	6	26	26					10	3	33	33	10	3	33	33	10	3	33	33	10	3	33	33
								5	7	17	12					10	4	28	28	10	4	28	28	10	4	28	28	10	4	28	28
								5	8	27	28					10	5	34	38	10	5	34	38	10	5	34	38	10	5	34	38
								6	1	16	11					11	2	28	31	11	2	28	31	11	2	28	31	11	2	28	31
								6	2	61	66					11	3	15	15	11	3	15	15	11	3	15	15	11	3	15	15
								6	3	21	16					11	4	47	51	11	4	47	51	11	4	47	51	11	4	47	51
								6	4	18	12					12	2	20	23	12	2	20	23	12	2	20	23	12	2	20	23
								6	5	20	17					12	3	33	33	12	3	33	33	12	3	33	33	12	3	33	33
								6	6	58	57					12	4	52	53	12	4	52	53	12	4	52	53	12	4	52	53
								6	8	51	49					12	5	16	15	12	5	16	15	12	5	16	15	12	5	16	15
								7	1	25	26					13	1	20	19	13	1	20	19	13	1	20	19	13	1	20	19
								7	2	62	61					13	2	38	40	13	2	38	40	13	2	38	40	13	2	38	40
								7	3	39	38					13	3	34	34	13	3	34	34	13	3	34	34	13	3	34	34
								7	4	31	34					13	4	27	24	13	4	27	24	13	4	27	24	13	4	27	24
								7	5	20	25					13	5	61	60	13	5	61	60	13	5	61	60	13	5	61	60
								7	6	15	11					14	1	28	27	14	1	28	27	14	1	28	27	14	1	28	27
								8	1	20	21					14	2	16	16	14	2	16	16	14	2	16	16	14	2	16	16
								8	3	30	32					14	3	42	40	14	3	42	40	14	3	42	40	14	3	42	40
								8	4	32	30					15	2	19	20	15	2	19	20	15	2	19	20	15	2	19	20
								9	1	36	41					15	3	35	30	15	3	35	30	15	3	35	30	15	3	35	30
								9	4	43	44					16	1	29	24	16	1	29	24	16	1	29	24	16	1	29	24
								9	5	42	41					16	2	32	34	16	2	32	34	16	2	32	34	16	2	32	34
								9	6	22	24					16	3	52	52	16	3	52	52	16	3	52	52	16	3	52	52

Table I. (continued)

K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC
7	3	41	41	1	3	127	119	8	2	55	54	17	6	33	34	5	6	71	72	13	1	64	62	2	2	77	71	9	3	58	44
7	4	39	39	1	4	92	89	8	3	101	99	18	2	20	23	5	7	44	45	13	2	15	13	2	3	114	120	9	5	21	19
7	5	24	24	1	5	24	29	8	4	15	13	18	4	32	36	5	8	34	31	13	4	28	27	2	4	89	79	9	6	28	28
7	6	14	14	1	6	21	19	8	5	46	47	18	5	16	16	6	1	17	9	13	5	55	53	2	5	27	30	9	7	27	28
7	8	22	23	1	7	27	27	8	6	41	43	19	1	31	27	6	2	29	26	13	6	44	41	2	6	19	15	9	8	14	17
8	1	51	48	1	8	52	47	8	7	39	38	19	2	22	20	6	3	37	36	13	8	23	22	2	8	24	21	10	2	48	44
8	3	41	41	1	9	22	20	8	8	18	18	19	4	19	17	6	4	123	121	14	1	47	44	2	9	18	17	10	3	90	93
8	4	33	32	1	10	17	15	8	9	43	43	19	5	17	20	6	6	28	31	14	2	21	18	2	10	16	13	10	5	32	29
9	1	62	62	2	1	154	154	9	1	26	25	20	1	26	23	6	8	35	33	14	3	42	44	3	1	76	74	10	6	21	23
9	2	45	44	2	2	72	69	9	3	67	67	20	2	18	19	6	9	15	12	14	4	28	26	3	2	88	84	10	7	23	21
9	3	12	13	2	3	36	33	9	4	44	44	20	3	21	20	6	10	50	49	14	5	27	29	3	3	53	54	10	9	23	21
9	4	13	11	2	4	74	71	9	5	41	43					7	1	145	138	14	6	36	33	3	4	14	7	11	1	47	44
9	5	17	20	2	5	73	72	9	6	16	18					7	2	93	96	14	7	42	41	3	5	25	24	11	2	53	51
9	7	27	27	2	7	35	35	9	8	25	23					7	3	88	79	15	1	36	37	3	6	42	40	11	5	47	47
10	1	21	18	2	8	31	29	9	9	27	29					7	4	12	3	15	2	22	22	3	7	51	49	11	6	14	16
10	2	26	25	2	9	26	23	10	1	105	110					7	5	44	41	15	3	57	55	3	9	32	28	11	7	16	18
10	3	30	33	3	1	67	69	10	4	32	29					7	6	29	29	15	4	26	23	4	1	84	83	11	8	15	16
10	5	37	40	3	3	58	56	10	5	49	48					7	7	44	46	15	5	20	20	4	2	11	14	12	2	38	36
10	7	14	12	3	4	98	97	10	6	28	24					7	9	14	5	15	7	35	33	4	3	35	37	12	4	30	32
10	9	25	22	3	5	96	94	10	7	36	34					8	1	120	121	15	8	22	21	4	4	58	57	12	7	23	21
11	1	37	38	3	6	39	37	11	1	25	25					8	2	102	97	16	1	21	20	4	5	77	75	12	8	37	34
11	2	45	45	3	7	20	20	11	2	59	63					8	3	38	37	16	3	28	29	4	7	25	24	12	9	25	25
11	3	19	19	3	8	31	30	11	3	57	60					8	4	12	9	16	4	32	31	4	8	17	20	13	1	50	51
11	4	22	24	3	9	20	19	11	4	68	69					8	5	63	57	16	5	34	36	4	10	19	17	13	2	13	12
11	6	14	17	3	10	31	32	11	5	17	17					8	6	50	53	17	1	15	14	5	1	20	11	13	3	17	17
11	7	21	23	4	1	30	28	11	8	44	43					8	7	14	13	17	2	51	48	5	2	41	40	13	4	34	35
11	8	15	13	4	2	36	38	12	1	20	16					8	8	32	34	17	6	34	35	5	3	51	47	13	5	21	28
12	1	24	26	4	3	137	137	12	2	49	49					8	9	25	27	18	1	18	16	5	4	89	92	13	6	25	25
12	4	30	28	4	4	39	36	12	4	33	36					9	2	91	91	18	3	22	23	5	5	50	55	13	7	20	28
12	5	15	15	4	5	56	53	12	5	19	19					9	3	65	66	18	4	38	38	5	6	31	28	14	2	18	16
12	6	24	22	4	6	40	39	12	6	65	65					9	4	77	76	19	1	40	35	5	8	47	43	14	3	25	25
13	1	22	20	4	7	41	41	13	1	22	22					9	5	42	42	19	2	21	20	5	9	31	29	14	4	21	23
13	2	23	26	4	9	56	54	13	2	40	43					9	6	45	43	19	3	28	28	6	2	117	117	14	5	33	36
13	3	53	52	4	10	16	14	13	3	55	59					9	7	32	33	20	1	29	33	6	3	29	26	15	2	26	26
13	4	27	29	5	1	92	92	13	5	21	25					9	8	35	30	20	2	21	19	6	4	23	25	15	3	32	33
13	7	24	24	5	2	104	101	13	6	21	20					10	1	75	77	21	2	21	19	6	6	96	100	15	5	16	13
14	2	19	23	5	3	37	32	13	7	31	32					10	2	37	37	21	2	21	20	6	8	21	24	15	7	17	19
14	3	23	22	5	4	29	22	13	8	28	30					10	3	73	77	21	3	22	19	6	9	17	12	16	1	41	39
14	5	21	19	5	5	46	48	14	1	43	43					10	4	44	45	21	4	19	21	6	10	21	19	16	2	18	22
15	1	15	16	5	6	44	46	14	2	57	56					10	5	19	21	7	2	11	13	7	2	11	13	16	3	16	37
15	5	20	20	5	7	30	32	14	3	27	27					10	6	22	22	7	3	88	76	7	3	88	76	16	7	27	27
16	1	27	25	5	8	18	18	14	4	33	32					10	7	57	58	7	4	43	43	7	4	43	43	17	2	20	15
16	3	27	26	6	1	20	14	14	5	21	21					10	8	41	40	8	4	47	52	7	5	36	35	17	3	15	28
17	4	32	29	6	2	105	105	14	7	23	24					10	9	24	19	8	6	23	18	7	6	22	23	17	4	32	31
17	6	19	15	6	4	116	116	15	1	27	26					11	1	38	35	8	8	39	36	7	7	31	28	17	5	20	28
18	2	32	29	6	5	32	28	15	3	18	16					11	2	14	11	8	10	42	39	7	9	31	28	17	6	28	28
				6	6	13	13	15	4	33	32					11	3	23	25	1	1	110	104	8	1	82	79	18	2	31	33
				6	8	33	32	15	5	60	58					11	4	55	56	1	2	13	16	8	2	21	20	18	6	17	13
				6	10	16	13	15	7	23	23					11	5	16	18	1	3	15	18	8	4	71	71	19	2	20	19
				7	1	98	101	15	8	51	52					11	6	28	25	1	4	66	63	8	5	43	41	19	3	28	29
				7	2	93	93	16	4	30	30					11	7	26	25	1	5	94	93	8	6	24	25	19	4	16	12
				7	3	57	53	16	6	16	20					12	1	16	12	1	6	35	31	8	7	15	16	20	1	23	23
				7	5	53	53	16	7	22	24					12	2	186	186	1	7	66	63	8	8	16	14	20	4	25	22
				8	10	39	35	17	1	19	21					12	3	60	61	1	9	25	18	8	9	22	22	21	1	34	31
				1	1	54	54	17	2	36	34					12	4	24	27	1	10	24	21	8	10	26	22	21	2	17	12
				1	2	105	104	17	5	16	15					12	5	45	46	1	11	18	16	9	1	83	83	21	3	21	18
																				2	1	28	28	9	2	57	61				

Table I. (continued)

K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC
H = -6				8	0	30	33	1	4	121	103	8	5	13	10	H = -6				6	6	124	129	13	4	14	13	1	3	39	38
0	2	76	61	9	1	27	25	1	5	54	52	8	6	28	23	6	10	42	45	13	5	34	36	1	4	50	56				
0	4	105	100	9	2	46	48	1	6	30	31	8	7	33	35	8	2	297	280	7	1	133	137	13	6	27	26	1	5	137	132
0	6	15	14	9	3	50	47	1	7	26	16	8	9	20	22	0	4	285	250	7	2	59	58	13	7	25	25	1	6	76	73
1	1	25	22	9	4	33	32	1	8	22	23	9	1	19	22	0	6	133	129	7	3	135	136	13	9	14	14	1	7	119	110
1	2	126	108	9	5	18	17	1	9	23	19	9	2	17	15	0	8	103	100	7	4	10	14	14	1	73	70	1	8	25	19
1	3	35	27	9	6	24	24	2	1	127	119	9	3	53	55	1	1	91	87	7	5	12	9	14	2	35	32	1	10	31	31
1	4	33	30	9	9	18	21	2	2	51	47	9	4	43	46	1	2	64	59	7	6	84	85	14	3	19	13	1	11	40	43
1	5	16	16	10	1	35	35	2	4	36	33	9	5	46	46	1	3	9	2	7	7	104	110	14	4	26	27	2	1	13	9
1	6	22	22	10	2	13	11	2	5	23	27	9	6	20	18	1	4	105	98	7	8	59	59	14	5	38	39	2	2	60	77
1	9	32	30	10	3	24	24	2	6	19	23	10	1	85	95	1	5	83	80	7	9	27	31	14	6	43	50	2	3	213	207
1	10	20	16	10	4	47	50	2	7	18	19	10	3	23	24	1	6	120	117	7	11	19	16	14	7	37	40	2	4	26	24
2	1	9	4	10	5	24	21	2	9	20	15	10	4	49	51	1	7	95	92	8	1	57	61	15	1	65	63	2	5	138	136
2	2	10	1	10	7	29	31	2	10	23	21	10	5	22	24	1	8	25	20	8	2	121	123	15	2	15	17	2	6	139	144
2	3	85	70	11	1	14	12	2	11	20	20	10	6	25	30	1	10	28	30	8	3	77	85	15	3	99	103	2	7	82	78
2	4	41	35	11	2	24	22	3	1	77	70	10	7	13	9	1	11	31	30	8	4	45	46	15	4	63	67	2	8	24	24
2	5	39	39	11	3	36	36	3	2	121	92	11	2	50	47	2	1	79	81	8	5	121	130	15	7	33	36	2	9	70	79
2	8	22	23	11	4	13	20	3	4	52	53	11	3	28	24	2	2	71	59	8	6	43	45	15	8	25	27	2	10	18	17
2	9	16	11	11	7	17	20	3	5	52	53	11	4	36	37	2	3	104	97	8	7	25	27	16	1	82	82	3	1	110	111
3	1	22	15	12	1	42	43	3	6	39	38	11	6	22	21	2	4	64	57	8	8	25	26	16	2	26	29	3	2	116	112
3	2	65	51	12	3	15	16	3	7	22	23	11	9	20	20	2	5	13	14	8	9	24	29	16	3	39	38	3	3	72	72
3	3	73	64	12	4	34	38	3	8	15	16	12	2	24	23	2	6	58	60	9	2	15	18	16	5	63	65	3	4	109	108
3	4	19	17	12	5	19	23	3	9	27	22	12	3	14	17	2	7	44	135	9	3	59	65	16	8	20	19	3	5	34	35
3	5	37	37	13	6	21	20	3	11	18	14	12	4	15	7	2	9	42	43	9	4	49	52	17	1	33	35	3	6	62	59
3	6	60	58	13	1	15	23	4	1	49	45	13	6	20	18	2	10	24	23	9	5	75	80	17	2	30	29	3	7	83	91
3	8	19	20	13	4	20	20	4	2	10	14	13	7	25	32	3	1	70	69	9	6	34	39	17	3	47	48	3	8	74	72
3	10	18	18	13	7	26	28	4	3	140	130	13	8	45	46	3	2	61	59	9	8	43	51	17	6	21	20	3	9	40	42
4	1	53	49	14	2	26	26	4	4	10	10	13	9	27	25	3	3	151	144	9	9	36	38	17	8	28	27	4	1	58	61
4	2	87	74	14	4	41	45	4	5	23	25	13	5	20	20	3	4	143	147	9	10	18	19	18	2	25	21	4	2	108	94
4	3	140	128	14	6	14	14	4	6	15	15	13	6	26	26	3	5	48	48	10	1	38	39	18	4	34	33	4	3	18	24
4	5	16	17	14	8	23	25	4	7	49	53	14	7	15	12	3	6	20	19	10	2	25	31	18	5	27	28	4	4	28	29
4	6	29	27	14	1	11	15	4	9	13	11	14	1	27	28	3	7	54	52	10	3	97	103	18	6	14	18	4	5	47	47
4	7	20	23	15	3	16	16	5	1	11	15	14	2	40	40	3	8	66	71	10	4	48	50	19	1	31	32	4	6	13	18
4	9	26	24	15	5	16	13	5	2	53	52	14	3	27	38	3	9	45	47	10	5	23	28	19	2	15	16	4	7	114	117
5	1	143	135	15	7	37	36	5	3	13	14	14	4	18	11	3	10	29	33	10	6	19	17	19	3	38	35	4	8	48	43
5	2	28	28	15	9	21	27	5	4	16	17	15	5	18	20	4	1	179	169	10	7	71	77	19	4	26	28	4	11	42	41
5	3	30	32	15	11	25	23	5	5	18	17	15	1	54	59	4	2	122	118	10	9	40	45	19	6	30	27	5	1	31	29
5	5	12	11	16	13	25	23	5	6	29	28	15	2	23	25	4	3	94	90	10	10	18	13	19	7	35	32	5	2	105	105
5	6	13	10	16	1	21	21	5	7	19	12	15	4	28	30	4	4	29	30	11	1	36	34	20	1	22	20	5	3	43	44
5	7	16	20	16	3	26	23	5	8	23	22	16	5	21	24	4	5	174	179	11	2	25	26	20	2	50	48	5	4	165	178
5	8	24	27	16	4	13	14	6	1	47	39	16	6	13	16	4	6	26	30	11	3	18	16	20	5	33	33	5	5	82	88
6	1	57	48	17	1	55	55	6	2	64	61	16	7	19	23	4	8	62	61	11	4	108	110	21	4	15	6	5	6	41	42
6	2	23	15	18	4	20	20	6	4	85	86	17	1	20	19	4	9	40	45	11	5	77	77	21	5	30	28	5	8	71	79
6	4	39	39	19	1	17	17	6	6	17	26	17	2	26	25	5	1	128	125	11	6	91	97	22	1	17	17	5	9	41	45
6	8	18	26	19	5	23	23	6	8	16	13	18	2	21	24	5	2	66	65	11	7	33	34	22	2	17	15	5	10	48	54
7	1	35	31	21	3	24	21	6	10	30	34	18	4	35	37	5	3	179	179	11	8	19	22	22	3	24	22	5	11	21	24
7	2	36	32	22	1	21	17	7	1	60	63	19	1	19	17	5	4	12	5	12	1	20	18	6	1	13	11	6	2	192	202
7	3	16	18					7	2	36	36	19	5	14	12	5	6	44	41	12	2	132	139								
7	5	44	43					7	4	43	45	19	6	16	16	5	7	75	81	12	3	34	39								
7	6	34	38					7	5	17	12	20	1	19	21	5	8	78	87	12	4	92	100								
7	9	20	19					7	7	17	11	20	2	14	12	5	9	25	24	12	6	54	53								
8	2	48	43					7	8	39	39	21	3	26	23	5	11	17	14	12	8	56	59								
8	3	46	46					8	1	49	50	22	1	26	24	6	1	10	1	13	1	37	38								
8	4	21	20					8	2	64	64					6	4	41	45	13	2	51	52								
8	7	26	30					8	3	53	53					6	5	49	53	13	3	13	15								

Table I. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
7	3	44	48	14	1	22	29	1	4	66	62	7	1	108	117	14	2	33	31	1	9	19	17	18	3	11	15	3	7	28	29
7	4	123	132	14	2	71	71	1	5	50	51	7	2	41	43	14	3	48	47	2	1	7	9	10	5	32	32	3	8	21	28
7	5	57	62	14	3	73	74	1	6	37	40	7	3	80	88	14	4	36	35	2	4	18	17	10	7	33	35	3	9	20	26
7	6	44	48	14	5	22	18	1	7	22	22	7	4	64	67	14	5	42	45	2	5	24	28	11	1	24	25	4	1	70	71
7	7	13	16	14	6	66	67	1	8	65	67	7	5	128	137	14	6	22	22	2	6	48	41	11	4	12	15	4	2	116	111
7	8	41	40	14	7	19	18	1	9	23	25	7	6	17	23	14	7	26	27	2	7	25	26	11	5	27	27	4	3	52	52
7	9	42	41	14	8	40	41	1	10	14	12	7	8	17	17	15	1	76	77	2	8	12	9	11	6	20	26	4	4	43	49
7	10	25	26	15	1	64	66	2	1	50	46	7	9	43	44	15	2	45	46	2	11	21	19	12	1	45	47	4	5	116	124
7	11	31	29	15	2	26	29	2	2	85	73	7	10	22	21	15	3	25	26	3	1	30	26	12	2	12	7	4	7	28	25
8	1	68	70	15	3	42	40	2	3	41	41	7	11	24	23	15	5	52	52	3	3	13	6	12	6	19	13	4	8	16	14
8	2	12	5	15	4	20	31	2	4	80	76	8	1	98	106	15	6	27	26	3	4	60	52	12	9	14	11	4	11	16	14
8	4	53	53	15	5	20	21	2	5	95	98	8	2	26	27	15	7	32	35	3	5	38	37	13	1	17	15	5	1	18	14
8	5	83	86	15	6	14	14	2	7	45	47	8	3	115	125	15	8	15	11	3	6	26	27	13	2	27	24	5	2	54	56
8	6	68	71	15	7	17	21	2	8	35	37	8	4	62	66	15	9	18	15	3	7	25	24	13	3	45	46	5	3	66	78
8	7	45	42	15	8	19	16	2	9	24	28	8	5	27	31	16	1	57	58	3	8	27	28	13	7	13	9	5	4	98	106
8	8	39	38	15	9	28	28	2	11	31	29	8	6	61	63	16	3	58	58	3	10	19	15	13	9	15	9	5	5	17	13
8	10	27	27	16	1	38	38	3	1	182	164	8	7	79	80	16	4	17	15	4	1	37	36	14	1	50	51	5	6	30	32
9	1	151	160	16	2	62	65	3	2	130	129	8	10	34	35	16	6	20	19	4	2	8	10	14	4	13	17	5	7	26	28
9	2	68	72	16	5	24	26	3	3	25	16	8	11	17	17	17	1	15	17	4	3	58	54	14	5	27	28	5	8	18	18
9	3	96	104	16	6	30	27	3	4	10	11	9	1	64	63	17	2	16	16	4	5	55	51	15	2	12	14	6	1	30	36
9	4	73	74	16	7	46	43	3	5	58	62	9	1	64	63	17	3	17	13	4	5	55	59	16	4	14	15	6	2	61	75
9	5	67	77	16	8	20	19	3	6	108	108	9	2	26	31	17	4	15	16	4	7	23	26	16	5	13	14	6	3	31	38
9	6	64	67	17	2	47	49	3	7	41	45	9	3	27	31	17	6	16	13	4	8	13	18	17	2	25	22	6	4	78	68
9	7	88	91	17	3	14	11	3	8	35	32	9	4	15	14	17	7	23	25	4	11	15	9	17	3	14	7	6	5	46	53
9	8	70	71	17	4	76	73	3	9	21	22	9	5	53	58	18	1	31	28	5	1	17	19	18	2	15	15	6	8	19	22
9	9	15	20	17	5	24	24	3	10	30	34	9	6	54	59	18	2	15	15	5	2	111	112	18	4	22	20	6	10	28	18
10	2	41	41	17	8	39	37	3	11	32	32	9	7	28	27	18	3	35	31	5	3	28	32	19	2	13	8	7	1	12	22
10	3	133	140	18	2	85	84	4	1	126	124	9	8	31	32	18	6	17	16	5	6	34	37	20	2	14	12	7	2	28	28
10	4	22	24	18	3	14	14	4	2	55	51	9	10	15	15	18	7	17	14	5	7	15	18	20	3	16	12	7	3	51	50
10	5	109	115	18	6	46	47	4	3	120	120	10	1	52	51	19	1	28	32	5	8	13	15					7	4	75	77
10	6	50	52	19	3	25	22	4	4	69	74	10	2	21	23	19	2	30	30	6	1	14	20					7	5	29	29
10	7	48	50	19	4	18	21	4	5	17	17	10	3	20	22	19	3	21	18	6	2	18	26					7	6	32	32
10	8	20	23	19	6	17	15	4	6	41	46	10	4	33	34	19	4	27	24	6	3	31	31					7	7	34	33
10	9	45	48	20	1	19	20	4	7	104	109	10	5	50	52	19	5	50	48	6	4	61	67					8	1	20	19
11	1	78	84	20	3	21	24	4	8	16	14	10	6	36	37	20	1	19	19	6	7	17	17					8	2	54	54
11	2	17	22	20	4	21	20	4	9	47	49	10	7	15	13	20	3	36	36	6	8	20	24					8	3	51	52
11	3	62	63	20	5	45	42	4	10	14	19	10	8	16	11	20	4	21	21	7	1	13	23					8	4	35	35
11	4	41	44	20	6	22	21	4	11	22	26	11	2	141	145	21	1	16	16	7	2	9	13					8	5	65	71
11	5	38	45	21	1	62	60	5	1	91	90	11	3	41	40	21	5	17	17	7	3	38	38					8	6	38	38
11	6	45	44	21	3	38	39	5	2	23	22	11	4	65	68	22	4	27	22	7	6	33	31					8	7	22	23
11	7	45	47	21	4	16	12	5	3	42	42	11	6	44	42	22	5	18	18	8	1	32	32					8	8	18	19
11	8	24	19	21	5	27	27	5	4	57	60	11	8	42	44	23	2	35	32	8	2	19	13					9	1	44	42
12	1	24	22	22	2	17	16	5	5	71	74	12	2	26	26					8	3	68	66					9	2	42	39
12	2	61	65	22	3	33	29	5	6	22	24	12	3	17	16					8	4	25	23					9	3	68	71
12	3	53	55	23	1	18	15	5	7	34	35	12	4	95	100					8	5	44	44					9	4	18	19
12	4	75	73	23	3	17	15	5	8	17	18	12	5	71	73					8	6	16	15					9	5	25	23
12	8	22	21					5	9	31	36	12	7	19	17					8	7	16	12					9	7	16	12
12	9	24	25					5	10	19	16	12	10	36	33					8	8	24	21					9	8	21	23
12	10	34	30					5	11	27	30	13	2	35	38					9	1	15	9					10	1	31	29
13	1	134	139					6	1	28	26	13	3	12	12					9	2	34	29					10	2	30	25
13	2	13	13					6	2	58	63	13	4	33	35					9	3	39	42					10	3	32	31
13	3	32	35					6	3	48	50	13	5	27	28					9	4	29	26					10	4	36	39
13	4	52	49					6	4	51	54	13	7	16	20					9	5	37	43					10	5	12	13
13	5	82	82					6	5	11	9	13	8	24	23					9	6	13	13					10	10	14	18
13	6	35	37					6	7	24	24	13	9	21	23					9	10	24	21					11	1	31	36
13	7	63	66					6	8	21	22	14	1	21	22					10	1	9	8					11	2	18	19

Table I. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
11	3	23	19	1	10	33	31	0	3	22	18	16	1	16	24	3	1	291	319	0	5	21	20	15	5	72	75	2	1	320	345	2	1	320	345
11	4	24	29	1	11	44	41	0	4	19	20	16	2	48	49	3	2	23	12	0	6	60	64	15	6	39	41	2	2	100	171	2	2	100	171
11	5	24	26	2	1	108	116	0	5	65	67	16	3	12	7	3	3	62	61	0	7	80	82	15	7	38	38	2	3	123	116	2	3	123	116
11	6	50	59	2	2	12	23	0	6	15	10	16	4	19	20	3	4	79	81	0	8	15	17	15	8	33	34	2	4	135	131	2	4	135	131
11	7	13	11	2	3	173	176	0	7	22	17	16	5	15	12	3	5	93	96	0	9	49	55	15	9	24	22	2	5	102	101	2	5	102	101
11	10	19	12	2	4	32	26	0	9	14	16	16	6	25	22	3	6	102	102	0	10	32	34	16	10	34	42	2	6	36	35	2	6	36	35
12	1	10	17	2	5	161	166	0	10	29	29	16	7	22	19	3	7	43	30	0	1	154	160	16	1	77	63	2	7	102	103	2	7	102	103
12	2	43	49	2	6	74	77	0	11	21	22	17	1	12	15	3	8	54	59	0	2	82	91	16	2	50	51	2	8	28	24	2	8	28	24
12	4	46	40	2	7	25	22	0	1	100	203	17	2	24	28	3	9	22	23	0	3	34	32	16	3	125	130	2	10	43	42	2	10	43	42
12	5	23	23	2	8	37	35	0	2	51	56	17	4	64	50	3	11	32	33	0	4	33	37	16	4	22	21	2	11	51	49	2	11	51	49
12	7	19	25	2	9	57	52	0	3	126	142	17	6	19	18	4	0	234	251	0	5	36	41	16	5	54	55	3	0	154	155	3	0	154	155
12	8	19	10	2	10	22	22	0	4	52	53	17	8	33	33	4	1	316	349	0	6	54	56	17	1	52	50	3	1	48	50	3	1	48	50
13	5	16	21	2	11	15	14	0	5	47	52	18	1	23	23	4	2	276	292	0	7	37	39	17	2	36	43	3	2	89	70	3	2	89	70
13	6	15	12	3	1	118	130	0	6	26	26	18	2	87	89	4	3	266	282	0	8	20	32	17	3	17	19	3	3	169	161	3	3	169	161
13	7	15	14	3	2	144	156	0	7	63	62	18	3	20	26	4	4	73	70	10	0	64	64	17	4	24	23	3	5	63	63	3	5	63	63
14	1	12	17	3	3	68	69	0	8	18	19	18	6	48	48	4	6	70	70	10	1	67	68	17	5	36	40	3	6	88	89	3	6	88	89
14	2	13	12	3	4	124	125	0	9	20	19	18	8	25	23	4	7	101	111	10	2	57	63	17	7	32	32	3	8	31	32	3	8	31	32
14	5	20	17	3	5	23	17	0	10	15	13	19	4	31	27	4	8	15	20	10	3	14	18	18	0	13	6	3	9	30	27	3	9	30	27
14	7	25	20	3	6	20	20	10	2	44	43	19	6	23	20	4	9	64	67	10	5	60	64	18	1	32	42	3	10	38	34	3	10	38	34
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15	3	33	30	3	8	22	12	10	5	104	107	20	3	21	25	4	11	23	21	10	7	25	34	18	6	28	28	4	0	19	11	4	0	19	11
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15	7	15	15	3	10	10	11	10	8	24	26	21	1	48	43	5	2	110	100	10	10	20	16	19	1	64	60	4	3	36	33	4	3	36	33
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16	1	17	9	4	2	177	175	11	1	116	121	22	2	16	17	5	4	92	104	11	2	267	204	19	3	21	21	4	7	12	10	4	7	12	10
16	2	25	21	4	3	105	111	11	2	26	29	22	3	27	21	5	5	159	172	11	3	67	73	19	4	34	33	4	8	14	17	4	8	14	17
16	3	14	11	4	4	50	59	11	3	36	40	22	5	25	24	5	6	54	56	11	4	93	95	19	5	54	50	4	9	18	16	4	9	18	16
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16	6	10	10	4	10	17	18	11	7	41	44	23	4	36	36	5	11	36	36	11	7	49	50	20	3	40	36	5	1	99	105	5	1	99	105
16	7	17	16	4	11	19	18	11	10	19	20	23	5	42	42	6	0	422	440	11	9	30	32	20	4	36	34	5	2	100	179	5	2	100	179
17	6	14	14	5	1	48	52	12	4	36	36	23	6	156	148	6	1	156	148	11	10	22	23	20	6	30	30	5	3	15	18	5	3	15	18
18	1	16	9	5	2	64	66	12	7	17	16	0	1	7	0	6	2	139	132	12	0	380	394	21	2	19	24	5	4	18	6	5	4	18	6
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18	5	19	20	5	4	215	227	12	9	27	23	0	4	194	191	6	4	97	95	12	2	116	123	22	4	18	21	5	6	130	143	5	6	130	143
19	3	18	19	5	6	34	41	12	10	16	16	0	6	134	130	6	6	23	24	12	3	37	36	22	5	20	19	5	7	42	37	5	7	42	37
19	6	16	16	5	8	47	46	13	1	150	153	0	8	19	16	6	7	19	17	12	4	106	105	23	2	49	49	5	8	52	50	5	8	52	50
20	1	13	10	5	9	24	26	13	2	58	59	0	10	113	108	6	8	26	29	12	6	89	95	23	4	23	23	5	9	26	27	5	9	26	27
20	5	18	17	5	10	34	30	13	3	83	88	1	1	135	149	6	9	16	13	12	10	60	58	24	0	38	29	6	0	204	217	6	0	204	217
21	1	17	16	5	11	19	22	13	4	42	41	1	2	380	401	6	10	37	39	13	1	29	29	24	1	20	10	6	1	20	10	6	1	20	10
21	3	15	13	6	1	131	139	13	5	31	20	1	3	235	204	7	1	352	355	13	2	66	69	24	2	66	69	6	2	132	126	6	2	132	126
				6	2	224	236	13	6	20	19	1	4	95	94	7	2	81	89	13	3	55	53	24	3	55	53	6	3	10	9	6	3	10	9
				6	3	26	25	13	7	49	46	1	5	166	153	7	3	54	52	13	4	30	36	0	2	50	43	6	4	308	315	6	4	308	315
				6	6	148	158	13	9	14	11	1	6	55	53	7	4	138	142	13	5	28	28	0	4	99	94	6	5	24	20	6	5	24	20
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				7	1	113	120	14	2	73	82	1	9	27	29	7	6	13	8	14	0	20	21	0	8	21	19	6	8	51	52	6	8	51	52
				7	2	52	41	14	3	70	72	1	10	26	24	7	7	33	35	14	3	52	52	1	1	101	91	6	10	45	45	6	10	45	45
				7	3	15	10	14	5	49	45	1	11	24	24	7	8	28	27	14	4	32	28	1	2	35	38	7	0	72	86	7	0	72	86
				7	4	195	204	14	6	45	45	2	1	15	14	7	9	42	42	14	5	22	26	1	3	150	130	7	1	28	34	7	1	28	34
				7	5	38	41	14	8	22	19	2	2	86	76	7	10																		

Table I. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
7	10	15	13	13	9	40	45	2	1	40	44	9	5	13	15	0	0	31	24	0	5	13	14	1	1	142	123	7	6	22	21
0	0	70	60	14	0	73	73	2	3	108	105	9	7	14	9	0	10	15	14	0	6	34	33	1	2	136	129	7	7	30	36
0	1	15	19	14	1	84	81	2	4	31	28	9	10	18	18	1	0	10	10	9	0	69	66	1	4	104	101	7	0	34	36
0	2	40	53	14	2	47	48	3	0	92	96	10	0	17	19	1	1	22	15	9	1	20	17	1	5	33	37	7	9	23	21
0	3	21	20	14	3	50	50	3	1	93	83	10	1	30	34	1	2	10	11	9	3	37	36	1	6	34	29	7	10	18	12
0	4	22	22	14	4	72	70	3	2	34	35	10	2	25	19	1	3	16	8	9	5	17	15	1	8	86	84	0	0	93	93
0	5	17	19	14	5	17	15	3	3	34	34	10	3	30	39	1	4	10	6	9	6	13	8	1	10	33	30	0	1	60	62
0	7	15	18	14	6	26	24	3	4	39	36	10	4	24	24	1	5	12	13	9	7	29	29	2	0	89	70	0	2	72	71
0	0	14	11	14	7	46	44	3	5	13	6	10	5	15	12	1	6	50	50	10	0	41	39	2	1	55	54	0	3	141	147
0	9	24	24	14	8	19	19	3	6	18	24	11	0	17	7	1	7	24	25	10	1	12	9	2	2	26	19	0	4	51	83
0	10	17	17	15	2	16	20	3	7	31	31	11	1	17	20	1	9	14	11	10	3	70	73	2	4	57	48	0	6	63	64
9	0	39	40	15	3	19	22	3	0	16	22	11	2	17	21	2	0	17	26	10	4	11	9	2	6	13	10	0	7	64	66
9	1	22	27	15	5	17	19	3	9	18	17	11	3	37	37	2	1	36	20	10	5	50	52	2	7	16	16	0	9	31	30
9	2	34	34	16	1	14	14	3	10	25	24	11	4	14	17	2	3	125	113	11	1	26	25	2	9	28	25	0	10	29	27
9	3	95	96	16	4	36	33	4	1	85	83	11	5	19	20	2	4	16	11	11	2	17	19	3	0	72	65	0	0	34	34
9	5	116	122	16	6	13	14	4	2	111	100	11	6	50	51	2	5	71	72	11	4	16	13	3	1	184	160	0	1	43	42
9	6	53	55	17	2	82	80	4	3	15	16	12	0	10	14	2	6	11	7	11	5	36	34	3	2	112	104	0	2	19	19
9	0	26	26	17	3	12	13	4	4	14	16	12	1	36	37	2	7	27	28	11	6	27	26	3	4	57	60	0	3	18	18
9	9	39	42	17	6	50	50	4	5	103	106	12	2	32	40	2	8	30	32	11	7	25	26	3	5	81	79	0	4	45	47
9	10	36	33	17	7	15	18	4	6	15	17	12	3	36	45	2	9	15	9	12	2	16	17	3	6	32	30	0	5	74	73
10	0	33	42	17	0	29	31	4	7	31	28	12	4	55	55	3	0	60	46	12	3	28	31	3	7	51	51	0	0	26	26
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10	7	76	78	19	3	23	22	5	4	127	123	14	0	14	15	4	0	43	36	14	5	21	19	4	3	157	152	11	0	12	14
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10	9	18	19	20	1	30	30	6	7	33	31	14	7	14	8	4	2	68	65	15	1	20	26	4	5	44	44	11	3	12	11
10	10	17	16	20	3	18	16	6	1	36	42	15	3	25	22	4	3	45	45	15	2	13	9	4	6	64	69	11	4	84	84
11	0	80	95	20	4	15	10	6	2	44	49	15	5	18	22	4	5	26	24	15	3	14	16	4	7	104	101	11	5	13	11
11	1	77	76	21	3	38	32	6	3	14	21	15	6	17	16	4	6	17	15	16	8	28	19	4	9	71	71	11	6	36	36
11	2	28	28	21	5	45	44	6	4	121	117	15	7	14	14	5	0	23	31	16	1	12	14	4	10	22	20	11	7	25	25
11	3	74	80	22	1	31	29	6	5	52	56	15	9	16	16	5	1	14	4	16	2	30	31	5	0	38	37	11	8	62	61
11	4	12	12	22	3	26	25	7	0	77	70	16	1	23	20	5	2	29	31	16	3	12	11	5	1	113	109	11	10	19	19
11	5	54	53	22	4	21	16	7	1	39	41	16	2	26	19	5	3	15	17	17	0	21	22	5	2	19	17	12	0	144	149
11	6	16	13					7	2	48	44	16	7	18	19	5	4	96	91	17	2	18	22	5	3	11	3	12	1	11	14
11	9	24	24					7	3	59	60	17	2	17	18	5	5	24	28	17	4	29	31	5	5	93	89	12	2	43	42
12	0	28	25					7	4	54	54	17	3	18	16	5	6	15	11	18	0	13	17	5	6	32	31	12	3	25	24
12	1	31	29					7	5	26	28	18	5	25	24	5	7	14	4	18	1	18	17	5	7	61	58	12	4	91	96
12	2	15	18					7	7	47	46	19	2	20	20	6	8	46	48	18	2	13	9	5	8	26	25	12	6	79	80
12	3	26	23					8	1	27	26	19	3	21	24	6	2	107	105	19	3	14	10	5	9	33	35	13	1	21	24
12	4	23	24					8	2	60	59	19	6	18	14	6	3	14	16	20	4	14	11	6	0	42	36	13	2	48	47
12	5	20	15					8	3	47	43	20	4	18	17	6	4	14	18	21	1	14	16	6	1	13	11	13	3	17	18
12	6	15	15					8	4	49	50	20	5	16	13	6	5	26	20	22	3	15	15	6	3	53	53	13	4	34	39
12	7	20	21					8	5	62	64	21	4	14	13	6	6	37	35					6	4	17	14	13	5	18	18
13	0	27	33					8	6	19	17	22	2	15	15	6	8	16	17					6	5	13	13	13	6	14	17
13	1	53	53					8	7	24	22	23	0	15	13	7	0	38	30					6	6	13	17	13	0	15	19
13	2	32	37					8	8	20	19	23	2	17	13	7	1	39	41					6	7	23	22	14	0	14	41
13	3	101	103					8	9	15	16					7	3	81	76					7	0	14	15	14	1	41	41
13	4	23	18					9	0	49	46					7	4	73	78												

Table I. (continued)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
15	2	31	26	2	7	177	167	8	8	23	21	16	8	51	51	9	0	124	122	16	5	68	67	3	7	25	21	3	7	25	21	3	7	25	21
15	4	29	29	2	8	22	19	8	9	16	19	16	1	26	28	9	1	63	65	16	7	43	38	3	10	31	32	3	10	31	32	3	10	31	32
15	5	49	50	2	9	27	27	8	10	21	17	16	3	23	19	9	2	127	128	17	0	20	18	4	8	58	44	4	8	58	44	4	8	58	44
15	7	38	38	2	10	43	41	9	0	36	35	16	4	22	19	9	3	70	78	17	1	21	15	4	1	14	7	4	1	14	7	4	1	14	7
15	8	17	18	2	11	43	39	9	1	40	42	16	8	25	24	9	4	22	22	17	2	36	37	4	2	10	7	4	2	10	7	4	2	10	7
16	8	34	34	3	2	104	105	9	2	80	77	17	0	75	77	9	6	141	142	17	3	46	44	4	4	36	38	4	4	36	38	4	4	36	38
16	1	49	49	3	3	118	104	9	3	129	131	17	1	15	14	9	8	19	23	17	4	20	17	4	5	40	38	4	5	40	38	4	5	40	38
16	3	62	62	3	4	54	49	9	5	125	124	17	2	94	89	9	8	25	27	18	0	32	32	4	6	22	16	4	6	22	16	4	6	22	16
16	4	22	21	3	5	89	87	9	6	75	70	17	6	50	43	9	9	38	34	10	0	21	24	4	8	19	21	4	8	19	21	4	8	19	21
16	5	16	18	3	6	109	96	9	7	20	18	18	0	73	74	9	10	45	38	10	1	31	29	5	0	107	105	5	0	107	105	5	0	107	105
16	6	20	18	3	7	17	13	9	8	31	28	18	1	17	17	4	0	18	14	10	2	45	47	5	1	52	51	5	1	52	51	5	1	52	51
16	7	31	34	3	8	40	36	9	9	43	42	18	2	34	32	4	1	263	245	10	4	34	38	5	2	60	55	5	2	60	55	5	2	60	55
17	2	16	19	3	9	38	38	10	0	51	51	18	3	20	17	4	2	118	110	10	5	25	26	5	3	41	36	5	3	41	36	5	3	41	36
17	5	16	14	3	10	20	13	10	1	153	154	18	4	71	72	4	3	38	41	10	6	15	16	5	4	56	53	5	4	56	53	5	4	56	53
17	7	21	18	4	0	42	36	10	2	30	31	18	6	30	26	4	4	29	26	10	7	16	13	5	6	52	47	5	6	52	47	5	6	52	47
18	0	19	20	4	1	13	14	10	3	150	145	18	7	15	9	4	5	186	185	11	0	139	140	5	7	25	28	5	7	25	28	5	7	25	28
18	3	31	28	4	2	39	38	10	4	77	74	19	0	39	39	4	6	25	21	11	2	71	72	5	8	18	21	5	8	18	21	5	8	18	21
18	7	18	12	4	3	54	48	10	5	55	57	19	2	29	29	4	7	111	108	11	4	97	98	5	10	28	27	5	10	28	27	5	10	28	27
19	1	45	44	4	4	20	16	10	7	95	93	20	1	48	40	4	8	60	57	11	5	31	33	6	0	59	68	6	0	59	68	6	0	59	68
19	2	31	31	4	5	20	21	10	9	26	30	20	3	23	21	4	9	26	23	11	6	102	103	6	1	59	51	6	1	59	51	6	1	59	51
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19	5	38	39	4	8	27	28	11	0	53	54	21	1	20	17	5	1	64	61	12	0	26	28	6	4	36	38	6	4	36	38	6	4	36	38
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20	3	41	38	5	2	193	190	11	3	64	67	21	5	39	34	5	4	42	44	12	3	74	75	6	8	47	47	6	8	47	47	6	8	47	47
20	4	21	18	5	4	30	26	11	4	47	47	22	1	52	47	5	5	52	50	12	4	134	140	7	0	15	12	7	0	15	12	7	0	15	12
21	5	22	18	5	5	38	36	11	5	85	84	22	3	43	40	5	6	23	24	12	5	14	17	7	2	57	55	7	2	57	55	7	2	57	55
22	0	31	28	5	6	144	140	11	6	24	27	12	6	24	23	5	7	73	73	12	6	24	23	7	3	34	29	7	3	34	29	7	3	34	29
22	2	18	14	5	8	91	93	11	9	24	24	12	8	64	66	5	9	43	46	12	8	64	66	7	4	37	36	7	4	37	36	7	4	37	36
23	2	35	33	6	0	185	188	12	1	36	36	12	0	97	93	6	0	97	93	13	0	92	98	7	6	13	9	7	6	13	9	7	6	13	9
24	8	29	25	6	1	11	5	12	2	31	29	12	1	11	14	6	1	11	14	13	1	69	72	7	7	30	31	7	7	30	31	7	7	30	31
				6	2	88	86	12	4	12	5	12	2	251	239	6	2	67	68	13	2	54	52	7	8	21	23	7	8	21	23	7	8	21	23
				6	3	20	13	12	6	17	17	12	4	295	287	6	4	48	50	13	3	17	14	7	9	21	24	7	9	21	24	7	9	21	24
				6	4	231	232	12	7	27	25	12	6	85	85	6	5	36	36	13	4	41	39	7	1	37	33	7	1	37	33	7	1	37	33
				6	5	45	49	13	8	72	70	13	0	103	105	6	6	42	47	13	5	50	52	7	0	11	11	7	0	11	11	7	0	11	11
				6	6	123	123	13	1	28	31	13	1	33	32	6	7	15	13	13	6	40	42	7	4	32	23	7	4	32	23	7	4	32	23
				6	7	13	14	13	2	85	84	13	2	200	184	6	8	17	22	13	7	15	12	7	6	15	10	7	6	15	10	7	6	15	10
				6	8	76	75	13	3	90	92	13	3	55	48	7	8	65	64	13	8	16	15	7	8	43	46	7	8	43	46	7	8	43	46
				6	9	14	11	13	4	21	17	13	4	150	143	7	1	33	34	13	9	29	30	7	1	84	83	7	1	84	83	7	1	84	83
				1	1	50	53	13	5	69	73	13	5	32	38	7	2	33	31	14	0	24	21	7	2	26	29	7	2	26	29	7	2	26	29
				1	2	12	15	13	6	27	27	13	6	89	84	7	3	152	153	14	1	27	28	7	3	12	8	7	3	12	8	7	3	12	8
				1	3	150	149	13	8	16	16	13	8	38	39	7	4	38	39	14	3	52	54	7	4	68	68	7	4	68	68	7	4	68	68
				1	4	42	38	13	9	58	54	13	9	152	149	7	5	72	71	14	4	26	27	7	5	14	18	7	5	14	18	7	5	14	18
				1	5	180	175	13	10	82	82	14	0	69	67	7	6	19	34	14	5	15	16	7	6	46	45	7	6	46	45	7	6	46	45
				1	6	36	37	14	1	119	119	14	1	25	21	7	7	88	89	14	6	23	25	7	7	31	38	7	7	31	38	7	7	31	38
				1	8	19	20	14	3	49	47	14	3	31	34	7	9	59	62	15	0	45	44	7	8	50	49	7	8	50	49	7	8	50	49
				1	9	69	68	14	4	85	85	14	4	40	36	8	0	42	40	15	1	59	60	7	9	61	79	7	9	61	79	7	9	61	79
				1	10	15	16	14	5	34	31	14	5	69	62	8	1	100	94	15	2	15	12	7	10	62	17	7	10	62	17	7	10	62	17
				1	11	32	30	14	6	28	26	14	6	31	30	8	2	79	83	15	3	30	29	7	11	13	11	7	11	13	11	7	11	13	11
				2	0	101	99	14	7	60	61	14	7	60	61	8	4	120	121	15	4	38	43	7	12	32	31	7	12	32	31	7	12	32	31
				2	1	218	209	14	8	19	20	14	8	19																					

Table I. (continued)

K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC	K	L	F0	FC
12	0	38	48	2	1	141	125	11	1	14	13	2	18	21	20	18	3	49	45	1	8	187	179	7	5	39	40	15	8	77	75
12	1	18	21	2	2	66	59	11	4	26	25	3	1	27	29	18	5	18	20	1	1	97	96	7	7	34	33	15	5	15	11
12	2	18	18	2	3	46	42	11	5	13	10	3	2	52	53	18	7	47	65	1	2	82	82	7	9	42	39	16	1	69	65
12	3	32	28	2	5	11	7	11	8	23	26	3	3	68	69	10	8	24	23	1	3	57	56	8	0	51	52	16	2	30	24
12	5	36	43	3	8	10	39	12	0	19	14	3	4	29	28	11	0	59	60	1	4	49	52	8	1	156	157	16	4	25	27
13	0	44	44	3	1	39	29	12	1	22	19	3	5	52	50	11	1	13	8	1	5	33	30	8	2	74	73	16	5	47	44
13	1	53	52	3	2	146	124	12	3	39	41	3	6	40	39	11	3	65	63	1	6	59	62	8	3	15	15	17	0	14	8
13	2	12	18	3	3	38	37	12	4	23	25	3	7	22	23	11	4	15	15	1	9	27	23	8	4	49	47	17	2	16	19
13	3	38	35	3	4	27	22	12	6	52	50	3	8	28	27	11	5	47	42	2	0	97	92	8	5	41	43	17	3	24	21
13	4	17	15	3	5	32	30	13	1	34	39	3	9	26	23	11	6	19	15	2	1	22	23	8	6	22	20	17	4	35	31
13	5	19	17	3	7	28	25	13	2	25	24	4	0	27	25	12	0	23	25	2	2	33	32	8	7	23	25	18	0	23	24
13	7	22	17	3	8	23	21	13	3	36	36	4	1	67	67	12	2	47	46	2	3	65	63	8	8	41	40	18	1	31	28
14	1	24	26	4	0	66	61	14	0	26	28	4	3	37	37	12	3	41	43	2	4	20	17	8	9	19	18	18	2	34	17
14	2	22	19	4	1	20	20	14	1	43	44	4	4	40	42	12	7	17	17	2	5	45	44	9	0	20	17	19	0	27	23
14	3	45	45	4	2	16	14	14	3	20	22	4	5	50	51	13	0	33	29	2	9	18	15	9	1	81	78	19	1	17	19
14	6	19	23	4	3	30	30	14	6	21	22	4	6	15	12	13	1	46	46	3	0	75	73	9	2	56	52	19	2	21	20
14	8	19	20	4	4	38	34	15	0	22	21	4	7	19	15	13	2	29	29	3	1	96	93	9	3	29	26	19	3	34	35
15	1	27	27	4	5	22	17	15	2	25	21	5	0	70	66	13	3	14	16	3	2	127	125	9	4	18	16	19	4	22	18
15	3	15	19	4	6	38	36	15	5	19	18	5	1	59	61	13	4	15	18	3	3	126	126	9	6	15	19	20	0	24	19
15	4	39	37	5	0	22	17	15	7	10	19	5	2	134	132	13	5	52	50	3	4	28	28	9	7	38	40	20	1	29	28
15	6	25	26	5	1	121	111	16	0	19	17	5	4	18	15	13	6	24	22	3	7	42	38	9	8	21	16	20	2	17	13
16	0	25	26	5	2	40	35	16	1	24	23	5	5	25	20	13	8	24	23	3	8	17	20	10	0	36	35	21	1	29	23
16	2	17	17	5	3	36	36	16	2	15	20	5	6	45	43	14	0	38	28	3	9	28	29	10	1	52	51				
17	0	33	31	5	4	13	13	16	4	16	18	5	8	42	43	14	1	36	34	4	0	45	39	10	2	47	48				
17	1	14	15	5	5	26	21	16	5	19	20	6	0	143	138	14	2	29	27	4	1	212	210	10	3	72	73				
17	4	38	41	5	8	23	23	16	6	15	15	6	1	13	12	14	3	28	28	4	2	81	80	10	4	16	16	8	8	143	140
17	6	22	19	5	9	15	15	17	1	34	32	6	3	16	17	14	4	38	29	4	3	29	27	10	5	25	25	8	2	17	19
18	0	17	18	5	10	22	17	18	1	25	25	6	4	142	139	14	6	27	29	4	4	67	64	10	8	20	22	8	4	76	78
18	1	27	25	6	0	24	21	18	3	16	14	6	5	12	14	14	7	28	26	4	5	74	76	11	0	124	122	8	6	26	28
18	2	23	20	6	1	87	74	19	5	15	17	6	6	42	41	15	1	25	21	4	6	15	13	11	1	50	51	8	6	46	42
18	5	21	23	6	2	47	44	20	1	19	13	6	7	14	12	15	2	14	12	4	7	48	58	11	2	79	78	1	0	12	7
18	6	16	15	6	3	38	33					6	8	43	41	15	3	20	21	4	8	25	23	11	3	21	20	1	1	91	95
19	1	16	10	6	6	21	24					7	0	67	64	15	5	27	26	4	9	19	21	11	4	34	38	1	2	93	91
19	2	18	18	7	0	37	37					7	1	38	39	16	1	15	11	5	0	67	63	11	5	34	31	1	3	119	117
19	4	15	16	7	2	35	35	8	8	52	50	7	2	69	68	16	4	30	29	5	1	15	7	11	6	65	65	1	4	60	59
20	1	28	20	7	3	29	29	8	2	130	132	7	5	22	28	16	5	16	11	5	2	47	46	12	0	38	35	1	5	21	19
20	3	16	18	7	4	31	31	8	4	37	29	7	6	46	46	17	0	31	29	5	3	116	106	12	1	16	11	1	7	68	67
21	1	24	21	7	5	44	46	1	0	94	83	7	7	19	21	17	2	56	55	5	4	48	45	12	2	92	92	1	9	29	25
22	0	19	14	7	7	40	40	1	1	70	69	7	8	16	14	17	4	18	18	5	5	32	27	12	4	69	71	2	0	48	38
22	3	17	13	7	9	15	17	1	3	95	89	8	0	37	36	17	6	30	27	5	6	16	14	12	6	14	14	2	1	84	85
				8	0	23	22	1	4	50	49	8	1	82	75	18	0	40	37	5	7	44	40	12	7	21	18	2	2	107	118
				8	1	72	62	1	5	76	69	8	2	43	44	18	4	36	33	5	8	25	23	12	8	55	52	2	3	88	86
				8	2	47	45	1	6	48	45	8	3	14	11	19	0	26	26	5	9	44	43	13	0	41	42	2	4	35	35
				8	5	26	29	1	7	19	17	8	4	14	13	19	2	16	13	6	0	141	137	13	1	28	27	2	5	88	87
				8	6	14	10	1	8	20	14	8	5	49	50	20	0	18	15	6	1	33	30	13	2	18	14	2	6	35	32
				8	7	19	18	1	9	45	46	8	6	27	27	20	1	35	34	6	2	54	53	13	4	26	24	2	7	16	14
				9	0	16	12	2	0	68	63	8	7	27	24	20	3	17	14	6	3	17	9	13	5	14	17	2	8	37	37
				9	1	30	31	2	1	78	80	9	1	22	21	21	3	27	22	6	4	31	32	13	6	34	33	2	9	33	36
				9	2	36	37	2	2	38	30	9	2	49	49	22	1	25	22	6	5	14	9	14	0	48	47	3	0	115	115
				9	4	17	15	2	3	64	71	9	3	77	73					6	6	46	44	14	3	26	24	3	1	126	124
				9	5	19	16	2	4	47	46	9	4	44	43					6	7	27	23	14	4	22	18	3	2	87	82
				10	0	45	44	2	5	21	16	9	5	23	24					7	0	98	88	14	5	49	47	3	3	28	33
				10	1	29	27	2	6	31	30	9	8	14	11	0				7	1	24	19	14	7	14	13	3	4	49	45
				10	2	12	13	2	7	52	54	9	9	34	33	0	2	169	169	7	2	21	21	15	0	24	24	3	5	33	33
				10	3	27	28	2	8	29	26	10	0	61	59	0	4	142	140	7	3	127	129	15	1	29	27	3	6	37	37
				11	0	15	16	2	9	16	14	10	1	97	96	0	8	104	101	7	4	61	58	15	2	47	46	3	7	25	22

Table I. (continued)

K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC	K	L	FQ	FC
4	0	72	72	11	2	59	59	2	2	43	42	11	0	20	22																
4	1	100	103	11	3	39	38	2	4	46	47	11	2	21	19																
4	2	16	12	11	4	15	14	2	5	31	34	11	3	20	19																
4	3	78	79	11	6	23	21	2	6	17	19	11	4	32	31																
4	4	30	26	11	7	43	43	3	0	76	70	12	0	48	40																
4	7	35	34	12	0	70	69	3	1	39	37	12	2	49	40																
5	0	114	116	12	1	30	38	3	2	13	15	12	5	28	27																
5	1	30	26	12	2	14	9	3	3	27	28	12	6	30	30																
5	2	10	14	12	4	36	37	3	4	40	40	12	7	16	14																
5	3	62	62	12	6	14	12	3	5	40	39	13	1	15	15																
5	4	102	101	13	1	49	51	3	6	20	20	13	2	24	23																
5	5	31	36	13	2	31	29	3	7	17	16	13	3	33	31																
5	6	52	51	13	3	59	59	3	8	35	40	13	4	15	15																
5	7	30	29	13	4	50	48	4	0	17	16	14	1	23	23																
5	8	15	10	13	5	23	19	4	2	10	16	14	3	10	17																
5	9	20	17	13	6	23	24	4	3	66	66	15	0	19	17																
6	0	70	72	13	7	37	37	4	5	25	24	15	1	33	35																
6	1	35	31	14	1	24	24	4	6	30	40	15	5	17	18																
6	2	165	167	14	2	49	40	5	0	52	51	16	3	32	31																
6	4	44	45	14	3	47	40	5	1	67	70	16	5	20	23																
6	6	61	63	14	4	20	29	5	2	43	40	17	0	19	20																
6	7	15	12	14	5	37	37	5	3	27	27	17	1	30	26																
6	8	65	64	14	6	23	22	5	5	24	25	17	2	17	14																
7	0	70	75	15	0	40	39	5	6	16	10	18	0	24	20																
7	1	19	14	15	1	34	32	5	7	30	31	19	1	15	15																
7	2	32	32	15	2	36	32	6	0	40	37	20	0	16	13																
7	3	60	60	15	3	32	27	6	1	11	2																				
7	4	49	48	15	6	21	21	6	2	52	52																				
7	5	14	15	16	1	32	31	6	4	37	36																				
7	6	21	18	16	2	23	21	6	8	23	20																				
7	7	21	20	16	3	31	38	7	0	32	30																				
7	8	17	14	17	0	44	44	7	1	53	52																				
8	0	50	57	17	4	46	46	7	2	39	38																				
8	1	73	72	18	0	16	17	7	3	34	35																				
8	2	19	16	18	1	34	31	7	4	16	13																				
8	3	56	53	18	2	52	51	7	5	29	28																				
8	4	39	36	19	2	15	6	7	7	30	42																				
8	8	20	17	19	3	22	18	8	0	54	52																				
9	0	75	72	21	0	17	12	8	2	43	45																				
9	1	07	92					8	3	33	33																				
9	2	40	46					8	5	17	16																				
9	3	55	57					8	6	32	34																				
9	4	33	32					8	7	25	25																				
9	5	20	18					8	8	20	20																				
9	6	35	34					9	0	52	51																				
9	7	45	47					9	1	17	13																				
10	0	35	35					9	2	12	2																				
10	1	71	69					9	3	15	16																				
10	2	40	47					9	4	32	33																				
10	3	35	35					9	5	16	15																				
10	4	14	19					9	6	27	26																				
10	5	74	75					10	0	19	22																				
10	6	33	30					10	1	56	56																				
10	7	21	19					10	2	13	6																				
11	0	22	20					10	4	24	22																				
11	1	41	38					10	5	17	16																				

Table I. (concluded)

K	L	FO	FC	K	L	FO	FC	K	L	FO	FC
9	1	22	22	7	1	37	38	4	2	17	12
9	2	30	28	7	2	24	25	5	0	45	46
9	3	38	39	7	4	28	16	5	2	42	47
9	4	35	33	8	1	34	35	6	0	43	44
9	5	35	38	8	2	15	18	6	2	18	24
10	1	65	69	8	5	20	20	7	0	25	26
10	3	26	20	9	0	15	11	H= 21			
10	4	31	31	9	1	18	15				
10	5	31	32	9	4	18	17				
11	0	24	20	10	0	18	18	1	0	47	53
11	1	16	8	10	1	16	11	1	1	23	24
11	2	24	27	10	2	16	15	2	0	16	14
11	3	30	29	10	3	32	32	3	0	33	35
11	4	31	33	11	0	46	47				
12	0	30	32	12	2	38	33				
12	1	25	23	13	0	23	19				
12	2	18	18	13	2	18	28				
13	2	26	28	14	0	24	23				
13	3	41	44								
14	1	36	35	H= 18							
14	3	22	25								
15	1	17	17	3	2	15	13				
16	0	17	18	5	0	19	22				
H= 17				H= 19							
0	2	61	67	0	0	43	46				
0	6	28	38	0	2	17	23				
1	0	61	57	0	4	29	30				
1	1	39	36	1	2	24	29				
1	2	17	16	3	0	17	15				
1	3	16	17	3	1	22	24				
1	4	17	20	4	0	23	23				
1	5	23	27	4	1	25	26				
1	6	18	16	4	3	38	42				
2	0	36	32	5	0	16	16				
2	1	19	21	5	1	20	22				
2	3	43	43	8	0	25	29				
2	4	17	15	8	1	19	23				
3	0	29	27	9	1	20	20				
3	2	35	35	9	2	16	18				
3	3	18	20								
3	4	28	30	H= 20							
4	0	14	10								
4	1	50	52	0	0	25	29				
4	2	16	13	0	2	23	28				
4	5	25	27	1	2	19	23				
5	1	21	19	1	3	35	38				
5	2	43	43	2	0	21	24				
5	3	15	8	2	1	68	68				
5	4	22	10	2	2	18	20				
6	0	46	46	2	3	28	31				
6	2	28	27	3	0	42	43				
6	3	18	16	3	1	22	20				
6	4	24	26	3	2	28	29				
7	0	19	21	4	0	19	8				

Table J. Observed (FO) and Calculated (FC) Structure Factors for Cu(DapsaH)·CH₃CN[illegible]

Table J. (continued).

K	L	F0	F0	K	L	F0	F0	K	L	F0	F0	K	L	F0	F0	X	L	F0	F0	K	L	F0	F0	K	L	F0	F0	K	L	F0	F0	
8	5	27	22	7	6	26	15	5	1	132	12A	2	0	13	16	16	2	23	23	16	J	25	26	14	2	23	25	16	0	26	27	
8	6	41	41	7	6	24	20	5	2	30	37	2	1	62	63	17	1	33	32	17	1	37	36	14	3	25	19	17	1	34	31	
9	1	53	56	8	0	43	41	5	3	23	27	2	2	45	50					19	4	25	19	15	4	33	32	18	2	27	20	
9	4	21	26	8	1	19	24	5	4	67	64	2	3	36	40	H= 3								16	3	27	29					
9	7	28	24	8	5	25	23	5	6	24	12	2	5	57	56					H= 4				17	1	27	29	H= 6				
10	1	38	42	9	1	41	44	5	7	36	33	3	0	47	39	0	0	162	158					17	4	25	21					
10	5	64	66	9	2	21	20	6	0	109	93	3	1	50	33	0	2	54	51	0	0	43	40					0	2	68	62	
11	2	41	43	9	4	21	20	6	1	93	84	3	2	40	44	1	0	19	11	0	2	112	113					1	0	24	22	
11	4	44	42	9	7	25	21	6	2	16	13	3	4	26	30	1	1	51	56	0	0	6	24	27					1	1	52	42
11	6	23	13	10	0	25	26	6	3	20	28	4	0	144	138	1	2	49	56	1	0	17	13					1	3	43	41	
12	1	41	41	10	1	59	61	6	4	31	28	4	1	22	28	1	3	89	84	1	1	46	44	0	2	44	46	1	4	31	28	
12	3	22	21	10	3	48	50	6	5	61	57	4	2	84	83	1	4	77	76	1	2	47	49	0	8	32	27	2	0	31	34	
12	6	28	26	10	4	23	24	7	0	32	26	4	3	19	5	2	1	50	52	1	3	64	63	1	0	31	28	2	1	28	23	
13	1	40	40	10	5	39	40	7	1	46	47	4	6	36	41	2	2	40	44	1	4	42	39	1	1	67	69	3	3	48	47	
14	2	26	23	10	6	24	17	7	2	81	81	5	0	29	31	2	3	113	114	2	2	25	23	1	2	78	74	2	5	40	36	
14	3	29	31	11	2	35	40	7	4	53	53	5	1	128	124	2	5	29	26	2	3	73	71	1	3	40	38	3	1	41	41	
15	2	23	26	11	3	21	24	8	0	32	33	5	2	52	54	2	7	28	22	2	5	44	45	2	0	29	27	2	2	38	33	
15	4	27	28	11	4	52	51	8	1	65	63	5	3	39	35	3	1	52	50	3	0	24	23	2	1	25	23	3	3	22	23	
				12	0	36	32	8	3	25	23	5	4	33	32	3	4	51	52	3	1	28	23	2	3	82	82	3	4	29	38	
				12	1	30	32	8	5	24	21	5	5	26	23	4	0	58	60	3	2	39	43	2	5	28	25	4	2	61	66	
				12	3	27	25	9	1	65	65	5	6	26	30	4	1	35	34	3	3	61	65	2	7	25	28	4	8	28	28	
				13	1	40	43	9	2	65	63	5	7	39	34	4	2	75	80	3	4	51	57	3	1	40	34	5	0	32	26	
				13	7	32	25	9	3	23	24	6	2	58	60	4	4	24	32	3	6	25	23	3	2	36	36	5	1	58	62	
				14	0	43	40	9	7	40	33	6	3	61	63	4	6	29	29	4	0	69	67	3	3	58	61	5	4	26	29	
				14	2	32	32	10	0	39	34	6	4	29	32	5	0	27	26	4	2	77	76	3	4	39	43	6	0	20	27	
				14	3	29	32	10	1	84	83	6	5	63	64	5	1	73	73	4	3	58	57	4	0	56	58	6	3	48	48	
				15	4	34	33	10	2	19	20	7	2	31	30	5	2	45	49	5	1	64	71	4	2	77	75	6	5	31	27	
				16	0	49	48	10	3	52	54	7	4	52	52	5	4	41	39	5	2	32	29	5	0	43	34	6	7	24	17	
				16	1	27	21	10	5	27	29	7	6	23	23	5	4	53	52	5	3	33	35	5	1	56	54	7	0	28	28	
				17	1	41	40	11	0	20	14	8	0	71	68	5	5	34	39	5	4	40	45	5	2	20	20	7	1	29	27	
				18	0	35	36	11	1	42	44	8	1	25	23	5	7	26	22	5	7	28	26	5	3	28	25	7	2	42	43	
								11	2	67	67	8	2	101	96	6	1	23	15	6	0	75	69	5	4	21	26	7	4	45	44	
								11	4	38	42	8	3	47	49	6	2	92	53	6	2	40	40	6	2	50	54	7	6	28	17	
								12	0	48	50	8	5	25	24	6	3	49	50	6	3	37	39	6	3	41	43	8	0	52	52	
								13	1	60	60	8	8	33	23	6	5	47	44	6	5	41	38	6	5	32	28	8	2	69	73	
								13	2	27	25	9	0	29	27	7	4	32	36	7	0	26	23	7	1	26	27	8	3	28	23	
								14	0	38	38	9	1	101	101	7	6	24	19	7	4	48	48	7	4	47	49	9	1	49	43	
								14	1	21	22	9	2	23	26	8	0	82	78	7	6	23	16	8	0	45	42	9	3	32	28	
								14	2	24	21	9	3	29	22	8	0	25	67	8	0	36	38	8	2	53	54	10	0	29	25	
								14	3	29	28	9	7	35	29	9	1	46	44	8	2	57	60	9	0	20	17	10	2	37	48	
								15	2	29	28	10	0	42	45	9	3	26	26	8	1	27	28	9	1	46	43	10	3	38	38	
								15	4	31	29	10	1	30	28	9	7	27	29	9	0	28	13	9	3	28	27	11	8	29	25	
								16	0	31	28	10	3	54	55	10	0	45	42	9	1	52	51	9	4	28	30	11	4	34	31	
								17	1	29	28	10	5	29	27	10	2	42	44	9	4	28	31	10	2	37	37	11	6	32	27	
								18	0	38	28	11	0	34	31	10	3	33	37	9	5	28	30	10	3	22	18	12	0	45	43	
												11	2	47	49	10	5	29	32	10	2	31	33	10	2	31	33	12	1	25	13	
												11	4	37	41	11	4	34	34	10	3	27	30	11	0	34	32	12	2	38	34	
												12	0	26	34	12	0	28	34	10	5	37	36	11	4	47	48	12	3	26	38	
												12	1	28	22	12	2	37	38	11	0	23	21	12	0	46	46	13	1	37	35	
												12	2	41	43	12	3	35	40	11	4	39	38	12	2	28	30	14	5	24	16	
												13	1	42	45	12	5	24	24	12	0	47	47	13	1	44	48	15	4	24	19	
												14	0	24	22	13	1	22	27	12	2	25	33	13	5	30	27	17	1	25	27	
												14	3	43	43	13	3	28	25	12	3	32	26	14	2	26	25					
												15	2	39	42	14	3	25	24	13	1	35	38	14	3	24	26					
												15	4	29	27	15	4	30	29	13	3	26	26	14	5	26	18					
												16	0	25	18	16	0	29	29	13	6	24	7	15	4	29	31	8	8	23	27	

Table J. (concluded).

K	L	F0	FC		K	L	F0	FC		K	L	F0	FC
0	2	48	51		3	4	34	34		8	2	26	28
1	1	27	28		4	0	63	63		9	1	29	28
1	2	22	29		4	2	36	34					
1	3	39	37		5	1	35	39	H= 11				
2	1	23	21		5	3	21	15					
2	3	44	47		6	5	32	31		0	0	50	48
2	5	33	27		7	1	24	19		1	0	32	29
3	1	24	5		8	0	54	53		3	0	28	25
3	3	33	28		9	0	27	30		3	1	24	25
3	4	30	31		10	5	26	22		4	0	37	36
4	0	66	65		11	0	25	27		4	2	26	26
4	1	31	31		12	0	33	30		5	1	24	27
4	2	53	56		13	1	33	34		6	2	29	29
5	1	37	38		13	3	25	21		9	3	26	24
5	2	27	26		15	1	26	22					
5	3	47	46										
6	0	33	33										
6	1	22	11										
6	3	43	44		0	0	50	52		0	0	24	20
6	5	28	30		0	2	54	54		0	2	38	37
6	7	24	12		0	4	40	44		2	1	29	27
7	0	28	27		1	0	24	26		2	5	27	19
7	1	23	18		1	1	38	41		4	2	23	20
7	4	46	48		2	1	26	8					
7	6	26	26		2	5	42	39	H= 13				
8	0	66	67		3	8	27	28					
8	1	21	8		3	1	28	32		0	2	28	27
8	2	52	54		3	2	38	38					
9	1	41	39		4	0	52	52					
10	1	28	27		4	3	33	39					
10	3	23	12		4	4	29	27					
10	5	26	25		5	0	21	18					
11	0	25	23		5	1	37	34					
11	6	25	23		6	5	37	29					
12	0	32	32		7	0	26	26					
12	2	32	36		7	2	27	28					
13	1	29	20		8	0	41	39					
17	1	25	21		9	1	25	34					
18	0	27	22		10	5	25	27					
					12	0	25	17					
					13	1	30	27					
					17	1	29	24					
				H= 8									
0	0	70	69										
0	2	47	49										
0	4	35	35										
1	0	27	25		0	0	56	55	H= 18				
1	1	38	37		1	0	24	24					
1	2	25	17		1	1	32	26					
1	3	48	53		2	1	24	4					
1	4	23	24		3	0	26	26					
2	1	31	27		3	2	25	23					
2	3	37	39		4	0	55	54					
2	5	25	26		4	2	32	33					
3	0	27	32		5	1	24	28					
3	1	43	43		6	4	25	22					
3	3	27	31		8	0	40	36					

Table K. Final Atomic Positional and Thermal Parameters for $[\text{Cu}(\text{EIA})]_4 \cdot \text{C}_4\text{H}_9\text{OH}^a$

ATOM	X	Y	Z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
CU1	.0937(1)	.0395(1)	-.0580(2)	4.48(7)	4.03(7)	3.62(7)	-.27(5)	1.49(5)	-.64(5)
CU2	.1675(1)	.0014(1)	-.2088(5)	5.51(7)	3.28(6)	3.00(6)	.12(5)	1.33(5)	-.07(5)
CU3	.2962(1)	.0237(1)	-.0641(5)	4.38(7)	3.99(6)	3.19(6)	-.02(5)	1.14(5)	.38(5)
CU4	.2087(1)	.2411(1)	-.1407(4)	5.12(8)	3.30(6)	4.00(7)	-.26(5)	.83(6)	-.00(5)
O11	.2025(5)	.1215(7)	-.0550(3)	5.0(4)	4.4(4)	3.0(3)	-.3(3)	1.5(3)	-.3(3)
O21	.1661(5)	-.0630(6)	-.1292(3)	5.4(4)	2.9(3)	3.5(4)	-.2(3)	1.7(3)	-.1(3)
O31	.2867(5)	.1131(7)	-.1396(4)	4.5(4)	4.3(4)	3.6(4)	-.1(3)	1.4(3)	.6(3)
O41	.1125(5)	.1396(6)	-.1868(4)	4.5(4)	3.6(3)	3.4(4)	.2(3)	.7(3)	-.1(3)
O12	-.0112(6)	-.0392(8)	-.1428(4)	4.3(4)	6.0(5)	6.2(5)	-.4(4)	1.7(4)	-1.2(4)
O22	.1691(7)	.0642(7)	-.2864(4)	9.6(6)	4.4(4)	4.0(4)	1.1(4)	3.5(4)	1.0(3)
O32	.3046(6)	-.0649(8)	.0085(4)	6.8(5)	6.2(5)	4.5(5)	.9(4)	2.4(4)	1.6(4)
O42	.3030(7)	.3442(8)	-.0994(5)	7.0(6)	4.6(5)	8.4(7)	-.8(4)	1.6(5)	-1.2(4)
N1	.0404(7)	.1282(9)	-.0487(5)	5.1(5)	4.9(5)	3.9(5)	.2(4)	1.7(4)	-.1(4)
N2	.2033(7)	-.1512(8)	-.2225(5)	7.3(6)	3.2(4)	3.4(5)	.5(4)	2.1(4)	-.4(3)
N3	.3982(6)	-.0419(9)	-.0758(4)	4.6(5)	4.8(5)	3.6(5)	-.7(4)	.8(4)	.3(4)
N4	.1159(7)	.3522(9)	-.1525(5)	6.3(6)	3.9(5)	4.6(6)	.3(4)	1.3(5)	-.0(4)

ATOM	X	Y	Z	B
C11	.1971(9)	.184(1)	.0032(6)	5.1(3)
C12	.1057(9)	.208(1)	-.0069(7)	5.5(3)
C13	-.073(1)	.204(2)	-.0100(8)	7.5(4)
C14	-.0396(9)	.124(1)	-.0521(7)	5.1(3)
C15	-.102(1)	.050(1)	-.0932(7)	5.8(3)
C16	-.0823(9)	-.024(1)	-.1345(7)	5.5(3)
C17	-.159(1)	-.095(2)	-.1746(8)	7.1(4)
C21	.1544(8)	-.186(1)	-.1345(6)	4.1(2)
C22	.2153(8)	-.231(1)	-.1683(6)	4.9(3)
C23	.269(1)	-.305(2)	-.2718(9)	8.2(4)
C24	.228(1)	-.184(1)	-.2696(7)	5.8(3)
C25	.223(1)	-.107(1)	-.3199(8)	6.4(3)
C26	.195(1)	.005(1)	-.3247(8)	6.6(3)
C27	.190(1)	.077(2)	-.386(1)	8.9(5)
C31	.3716(8)	.120(1)	-.1466(6)	4.8(3)
C32	.4166(9)	.003(1)	-.1318(6)	5.2(3)
C33	.524(1)	-.176(1)	-.0578(3)	6.9(4)
C34	.4467(9)	-.127(1)	-.0429(7)	5.0(3)
C35	.4289(9)	-.176(1)	.0084(7)	5.2(3)
C36	.3649(9)	-.144(1)	.0287(7)	5.5(3)
C37	.352(1)	-.207(2)	.0860(9)	8.3(5)

Table K. (Continued).

ATOM	X	Y	Z	B
C41	.0417(9)	.206(1)	-.226(6)	5.0(3)
C42	.0282(9)	.310(1)	-.1891(7)	5.5(3)
C43	.044(1)	.519(2)	-.1218(8)	7.3(4)
C44	.1246(9)	.450(1)	-.1198(7)	5.4(3)
C45	.208(1)	.489(1)	-.0814(7)	6.0(3)
C46	.287(1)	.441(1)	-.0747(8)	6.6(4)
C47	.374(1)	.501(2)	-.035(1)	9.6(5)
C1R	.447(4)	.424(5)	-.216(3)	5.7(12)
C2R	.386(4)	.445(6)	-.198(3)	6.4(14)
C3R	.460(5)	.421(7)	-.164(4)	8.5(19)
O1B	.521(5)	.511(7)	-.187(3)	13.2(21)
C4R	.432(5)	.362(6)	-.264(4)	7.4(17)

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4(B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}l^2c^{*2} - 2B_{12}hka^{*}b^{*} - 2B_{13}hla^{*}c^{*} - 2B_{23}klb^{*}c^{*})].$$

Table L. Final Atomic Positional and Thermal Parameters for $[\text{Ni}(\text{EIA})(\text{CH}_3\text{OH})]_4$.^a

Atom Name	X	Y	Z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ni(1)	0.1786(1)	0.17013(5)	-0.1011(1)	0.0044(1)	0.00116(3)	0.00329(8)	0.00022(5)	0.00022(8)	-0.00006(4)
Ni(2)	0.2134(1)	0.17748(6)	-0.3308(1)	0.0045(1)	0.00100(2)	0.00368(9)	0.00013(5)	0.00046(9)	0.00020(4)
Ni(3)	0.1390(1)	0.07276(5)	-0.2477(1)	0.00456(9)	0.00098(2)	0.00380(9)	-0.00019(5)	-0.0001(1)	0.00006(4)
Ni(4)	0.3674(1)	0.10829(5)	-0.1900(1)	0.0043(1)	0.00100(2)	0.0045(1)	0.00024(5)	0.0000(1)	-0.00008(4)
O(11)	0.0978(6)	0.1517(3)	-0.2328(6)	3.0(2)					
O(21)	0.2674(6)	0.1035(3)	-0.3220(5)	2.7(1)					
O(31)	0.2226(6)	0.0915(3)	-0.1197(5)	2.7(1)					
O(41)	0.3083(5)	0.1809(3)	-0.1970(5)	2.6(1)					
O(13)	0.1640(6)	0.2528(3)	-0.1230(6)	4.2(2)					
C(18)	0.0905(13)	0.2874(7)	-0.0685(12)	6.4(4)					
C(11)	-0.0127(9)	0.1697(5)	-0.2229(8)	3.6(2)					
C(12)	-0.0561(9)	0.1560(5)	-0.1142(9)	3.7(3)					
N(1)	0.0318(8)	0.1647(4)	-0.0384(7)	3.6(2)					
C(14)	0.0123(9)	0.1646(5)	0.0579(8)	3.5(2)					
C(13)	-0.107(1)	0.1541(5)	0.092(1)	4.7(3)					
C(15)	0.0935(9)	0.1733(5)	0.1307(8)	3.7(2)					
C(16)	0.2031(9)	0.1812(5)	0.1197(9)	4.0(3)					
C(17)	0.277(1)	0.1912(5)	0.209(1)	4.9(3)					
O(12)	0.2535(6)	0.1779(3)	0.0312(6)	3.8(2)					
C(28)	0.091(1)	0.1610(6)	-0.556(1)	5.6(3)					
O(23)	0.0839(6)	0.1574(3)	-0.4444(6)	3.8(2)					
C(21)	0.307(1)	0.0894(5)	-0.4221(9)	3.8(3)					
C(22)	0.374(1)	0.1343(5)	-0.4671(9)	3.7(2)					
N(2)	0.3218(7)	0.1831(4)	-0.4411(7)	3.3(2)					
C(24)	0.354(1)	0.2278(5)	-0.4829(9)	3.8(3)					
C(23)	0.445(1)	0.2261(6)	-0.563(1)	5.1(3)					
C(25)	0.306(1)	0.2756(5)	-0.4571(9)	3.9(3)					
C(26)	0.233(1)	0.2855(5)	-0.3872(9)	3.8(2)					
C(27)	0.202(1)	0.3430(5)	-0.360(1)	5.0(3)					
O(22)	0.1819(6)	0.2531(3)	-0.3268(6)	3.8(2)					
O(33)	0.2333(6)	0.0011(3)	-0.2723(6)	3.8(2)					
C(38)	0.208(1)	-0.0510(6)	-0.242(1)	5.7(3)					
C(31)	0.205(1)	0.0529(5)	-0.0450(9)	3.6(2)					
C(32)	0.080(1)	0.0364(5)	-0.048(1)	4.1(3)					
N(3)	0.0409(8)	0.0363(4)	-0.1529(7)	3.3(2)					

Table L. (Continued).

Atom Name	X	Y	Z	B or β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(34)	-0.053(1)	0.0145(5)	-0.177(1)	4.0(3)					
C(33)	-0.120(1)	-0.0129(6)	-0.094(1)	6.8(4)					
C(35)	-0.0930(9)	0.0150(5)	-0.275(1)	4.0(3)					
C(36)	-0.051(1)	0.0390(5)	-0.3633(9)	3.9(3)					
C(37)	-0.114(1)	0.0392(6)	-0.462(1)	5.5(3)					
O(32)	0.0409(6)	0.0625(3)	-0.3670(5)	3.4(2)					
O(43)	0.4293(7)	0.1231(3)	-0.0368(6)	4.1(2)					
C(48)	0.484(1)	0.0827(6)	0.020(1)	6.3(4)					
C(41)	0.3980(8)	0.2157(4)	-0.1853(9)	3.1(2)					
C(42)	0.496(1)	0.1969(4)	-0.243(1)	3.8(2)					
N(4)	0.5036(7)	0.1410(4)	-0.2388(8)	3.3(2)					
C(44)	0.590(1)	0.1157(5)	-0.266(1)	4.3(3)					
C(43)	0.692(1)	0.1466(6)	-0.299(1)	6.8(4)					
C(45)	0.596(1)	0.0594(5)	-0.268(1)	4.8(3)					
C(46)	0.520(1)	0.0262(5)	-0.241(1)	4.3(3)					
C(47)	0.541(1)	-0.0328(6)	-0.257(1)	6.0(3)					
O(42)	0.4227(6)	0.0365(3)	-0.2053(6)	3.7(2)					

^a The form of the thermal ellipsoid expression is:

$$\exp [-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl]$$

Table M. Atomic Positional and Thermal Parameters for the Complex $\text{Fe}_2(\text{DSALZ})_3$.^a

ATOM	X	Y	Z	U11	U22	U33	U12	U13	U23
FE1	-.0723(1)	.3168(1)	.5637(2)	1.89(8)	3.5(1)	2.57(9)	-.0(1)	.2(1)	-.8(1)
O1	-.1591(5)	.3366(8)	.4210(8)	2.7(5)	6.3(8)	3.8(6)	-.5(5)	1.1(5)	-1.7(6)
O2	-.0232(6)	.2189(9)	.0301(9)	4.4(6)	5.1(7)	2.9(6)	.4(6)	1.3(5)	-.3(6)
O3	-.0361(5)	.4265(6)	.3648(7)	2.6(5)	2.7(5)	4.1(6)	.5(4)	-.2(5)	-1.5(6)
N1	-.1291(5)	.3335(8)	.2347(9)	2.5(6)	2.2(7)	3.2(7)	.0(5)	-.1(5)	-.8(5)
N2	-.0943(5)	.314(1)	.1548(9)	2.5(5)	3.7(7)	2.6(7)	.9(6)	-.2(4)	-.6(7)
N3	.0143(6)	.2885(8)	.2740(9)	1.4(5)	2.5(6)	2.9(7)	-.2(5)	.1(5)	-.9(5)
C11	-.219(1)	.364(1)	.393(2)	2.1(8)	5.1	5.2	-.4(8)	.8(8)	-2.5(9)
C12	-.269(1)	.379(2)	.467(2)	3.0	10.0	9.2	-.9	.7	-6.4
C13	-.331(1)	.407(2)	.443(2)	3.4	11.5	9.4	-.8	.6	-7.1
C14	-.350(1)	.422(2)	.355(3)	2.5(9)	6.6	14.3	.7(9)	2.4	-5.2
C15	-.303(1)	.408(1)	.280(2)	3.6(9)	6.2	8.5	.3	1.1	-1.9
C16	-.2361(9)	.374(1)	.307(2)	1.4(8)	4.9	6.4	.9(8)	.5(9)	-1.5
C17	-.1930(3)	.356(1)	.226(1)	2.7(8)	1.7(8)	5.6	.2(6)	.6(8)	-.4(7)
C21	-.021(1)	.286(2)	-.021(1)	3.7(9)	7.2	3.3	-.3	-.7(8)	.0
C22	.013(1)	.285(2)	-.110(1)	6.8	10.8	2.5	-1.7	.6	-1.8
C23	.014(2)	.353(2)	-.164(1)	11.4	6.2	2.6	-3.0	.6	1.8
C24	-.014(1)	.424(2)	-.140(2)	10.3	7.5	4.3	-2.7	-.8	-.4
C25	-.050(1)	.431(2)	-.053(2)	6.1	7.9	4.4	-.9	-2.3	2.6
C26	-.0524(9)	.361(1)	.006(1)	3.8(9)	3.8	3.1(9)	-.4(9)	-1.0(7)	.2(9)
C27	-.0866(9)	.373(1)	.093(1)	3.5	3.9	4.1	.4(7)	.4(8)	-.3(8)

ATOM	X	Y	Z	D
C31	.0261(7)	.4561(9)	.354(1)	2.3(3)
C32	.0415(8)	.535(1)	.395(1)	2.9(4)
C33	.1052(9)	.569(1)	.386(1)	3.5(4)
C34	.156(1)	.528(1)	.333(1)	4.5(5)
C35	.1411(9)	.452(1)	.292(1)	3.7(4)
C36	.0780(8)	.415(1)	.307(1)	2.6(3)
C37	.0675(9)	.3338(9)	.264(1)	2.7(3)
OSLV	.23300	.25000	.25000	10.00
C1SLV	.24830	.25000	.25000	10.00
C2SLV	.31700	.23700	.29000	10.00

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4(B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}l^2c^{*2} - 2B_{12}hka^{*}b^{*} - 2B_{13}hla^{*}c^{*} - 2B_{23}k\ell b^{*}c^{*})].$$

Table N. Final Atomic Positional and Thermal Parameters for $[\text{Co}(\text{Dapo})(\text{DapoH})]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$.^a

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
CO1	0.00000	0.00000	0.00000	.00130(3)	.0044(1)	.00217(6)	-.00012(6)	.00018(3)	.00016(9)
CL1	.19969(7)	.3594(1)	-.3559(1)	.00241(5)	.0089(2)	.0068(1)	-.00071(8)	.00032(6)	.0002(1)
OH2	-.3818(2)	-.1506(5)	.2800(3)	.0032(1)	.0156(7)	.0067(3)	-.0009(3)	.0009(2)	-.0016(4)
N2	.1212(2)	.0204(4)	.1041(3)	.0016(1)	.0076(6)	.0039(3)	-.0003(2)	.0002(1)	.0007(4)
N1	-.0071(2)	.2399(4)	.3243(3)	.0019(1)	.0054(5)	.0045(4)	-.0004(2)	.0009(2)	.0000(3)
O1	-.0469(2)	-.0505(3)	.1409(2)	.0021(1)	.0071(4)	.0028(2)	-.0009(2)	.0005(1)	-.0004(2)
C1	.0458(3)	.3211(5)	-.0545(4)	.0026(2)	.0059(6)	.0049(4)	-.0003(3)	.0010(2)	.0009(4)
C2	.1690(3)	.1193(6)	.0266(4)	.0017(2)	.0092(7)	.0045(4)	-.0006(3)	.0005(2)	.0002(4)
C3	.1025(3)	.1881(5)	-.0899(4)	.0020(2)	.0072(6)	.0034(4)	-.0011(3)	.0008(2)	-.0002(4)

ATOM	X	Y	Z	B
HC1	.078(4)	.383(8)	-.481(6)	5.00000
HC1*	.004(4)	.366(8)	-.124(7)	5.00000
HC3	.133(4)	.223(8)	-.158(6)	5.00000
HC2	.201(4)	.220(9)	.079(6)	5.00000
HC2*	.207(4)	.044(8)	-.011(6)	5.00000
HBND	.003(5)	-.068(7)	.210(6)	5.00000

^a The form of the thermal ellipsoid expression is:

$$\exp [-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}\ell^2 - 2\beta_{12}hk - 2\beta_{13}h\ell - 2\beta_{23}k\ell]$$

Table O. Final Atomic Positional and Thermal Parameters for $[\text{Cu}(\text{Dapo})_2(\text{DapoH})_2]\text{I}_4 \cdot \text{CH}_3\text{OH}^a$

ATOM	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
I(1)	.4842(1)	.1457(1)	.29741(8)	.0060(1)	.00312(9)	.00270(5)	.00033(8)	.00003(5)	.00051(5)
I(2)	-.0234(1)	.3026(1)	.36494(8)	.0063(1)	.00334(8)	.00247(5)	.00027(8)	-.00048(5)	.00084(5)
I(3)	.0017(1)	.4408(1)	.12372(8)	.00417(9)	.00468(9)	.00231(4)	-.00014(8)	-.00046(5)	.00059(5)
I(4)	.3891(1)	.1425(1)	.02821(9)	.0097(2)	.0051(1)	.00267(5)	.0023(1)	-.00067(7)	-.00062(6)
Cu(1)	.1821(2)	.3078(2)	.0771(1)	.0053(2)	.0027(1)	.00149(6)	-.0013(1)	-.00081(8)	.00046(8)
Cu(2)	.2690(2)	.5150(2)	.1707(1)	.0055(2)	.0026(1)	.00138(6)	.0005(1)	-.00003(8)	.00015(8)
Cu(3)	.4995(2)	.4027(2)	.2515(1)	.0043(2)	.0036(1)	.00130(6)	-.0000(1)	-.00031(8)	-.00019(8)
O(1)	.292(1)	.4238(9)	.0937(6)	.0040(9)	.0021(7)	.0017(4)	.0008(7)	.0002(4)	.0002(4)
N(11)	.244(1)	.627(1)	.1015(8)	.007(1)	.002(1)	.0013(4)	.0007(9)	-.0005(6)	.0001(5)
N(12)	.169(1)	.358(1)	-.0199(8)	.006(1)	.003(1)	.0016(4)	-.002(1)	-.0008(6)	.0005(6)
O(2)	.336(1)	.4189(9)	.2398(6)	.005(1)	.0028(8)	.0013(3)	-.0002(7)	-.0001(4)	-.0001(4)
N(21)	.196(1)	.578(1)	.2459(8)	.006(1)	.004(1)	.0020(5)	.001(1)	.0005(6)	.0002(6)
N(22)	.490(1)	.439(1)	.3498(8)	.006(1)	.004(1)	.0014(4)	.000(1)	.0002(6)	-.0005(6)
O(3)	.702(1)	.242(1)	.1590(8)	.007(1)	.0037(9)	.0026(5)	.0008(9)	.0001(6)	.0004(5)
N(31)	.495(1)	.346(1)	.1563(7)	.006(1)	.0023(9)	.0012(4)	.0006(9)	.0001(6)	-.0006(5)
N(32)	.664(1)	.381(1)	.2693(8)	.004(1)	.007(1)	.0014(5)	-.000(1)	-.0003(6)	-.0002(7)
O(4)	.170(1)	.032(1)	.1490(9)	.008(1)	.004(1)	.0041(6)	-.0019(9)	-.0013(7)	.0013(6)
N(41)	.237(1)	.241(1)	.1671(8)	.006(1)	.003(1)	.0018(5)	-.0005(9)	-.0014(6)	.0006(6)
N(42)	.087(1)	.181(1)	.0504(9)	.006(1)	.005(1)	.0028(6)	-.003(1)	-.0010(7)	.0014(7)

ATOM	X	Y	Z	B
C(11)	.226(2)	.578(2)	.035(1)	2.6(4)
C(12)	.301(1)	.483(1)	.0353(9)	2.2(3)
C(13)	.270(2)	.416(2)	-.027(1)	2.8(4)
C(21)	.189(2)	.494(2)	.294(1)	3.6(4)
C(22)	.295(2)	.434(2)	.304(1)	2.5(3)
C(23)	.383(2)	.493(2)	.350(1)	3.0(4)
C(31)	.579(1)	.382(1)	.1181(9)	2.1(3)
C(32)	.696(2)	.352(2)	.1477(9)	2.4(3)
C(41)	.153(2)	.195(2)	.207(1)	3.4(4)
C(42)	.091(2)	.106(2)	.168(1)	3.4(4)
C(43)	.022(2)	.142(2)	.099(1)	4.6(5)
OSOLV	.671(2)	.179(2)	.026(1)	8.0(6)
CSOLV	.740(2)	.135(2)	-.010(1)	5.7(6)
H(11)	.15100	.55500	.02500	5.00000
H(11)	.24100	.62400	0.00000	5.00000
H(12)	.37500	.50700	.03600	5.00000
H(13)	.32900	.36800	-.03200	5.00000
H(13)	.25900	.45600	-.06800	5.00000

Table O. (Continued).

ATOM	X	Y	Z	B
H(21)	.13000	.44800	.27700	5.00000
H(21)	.17400	.52000	.33600	5.00000
H(22)	.28300	.36900	.32400	5.00000
H(23)	.36300	.49500	.39600	5.00000
H(23)	.38700	.56200	.33500	5.00000
H(31)	.57500	.45600	.11500	5.00000
H(31)	.56500	.35500	.07300	5.00000
H(32)	.74700	.37200	.11800	5.00000
H(33)	.73200	.47800	.20800	5.00000
H(33)	.80700	.38500	.23000	5.00000
H(41)	.10000	.24600	.21700	5.00000
H(41)	.18800	.16900	.25000	5.00000
H(42)	.04200	.07500	.19700	5.00000
H(43)	-.03100	.19200	.10900	5.00000
H(43)	-.02000	.08200	.08000	5.00000

^a The form of the thermal ellipsoid expression is:

$$\exp [-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl]$$

Table P. Final Atomic Positional and Thermal Parameters for Cu₂(Dapac)(OAc).^a

ATOM	X	Y	Z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
CU(1)	.16467(4)	.35363(4)	-.09870(4)	2.44(2)	2.60(2)	2.71(2)	.02(1)	.40(1)	.34(2)
CU(2)	.11207(4)	.16866(4)	.06943(4)	2.00(2)	2.66(2)	2.70(2)	-.02(1)	.22(1)	.35(2)
O(11)	.2399(2)	.4763(2)	-.1399(3)	3.6(1)	3.2(1)	4.4(1)	-.2(1)	1.2(1)	.7(1)
O(21)	.1366(2)	.1366(3)	.2240(2)	2.9(1)	4.8(1)	2.9(1)	-.2(1)	.35(9)	.7(1)
O(31)	.0874(2)	.2195(2)	-.0826(2)	2.4(1)	2.9(1)	2.8(1)	.06(9)	.14(9)	.28(9)
O(41)	.3147(2)	.2900(3)	-.0328(3)	2.6(1)	3.9(1)	5.5(2)	-.1(1)	.5(1)	1.4(1)
O(42)	.2782(2)	.1706(3)	.0911(3)	2.3(1)	5.2(2)	3.7(1)	.2(1)	.3(1)	1.3(1)
N(11)	.0149(3)	.4178(3)	-.1412(3)	2.9(1)	3.0(1)	2.8(1)	.1(1)	.1(1)	.2(1)
N(21)	-.0484(3)	.1366(3)	.0323(3)	2.6(1)	2.8(1)	3.0(1)	-.2(1)	.2(1)	.2(1)
C(11)	.2721(5)	.6506(4)	-.2073(5)	6.4(3)	3.4(2)	5.4(3)	-1.2(2)	2.2(2)	.5(2)
C(12)	.1901(4)	.5657(3)	-.1797(4)	4.8(2)	3.1(2)	2.6(2)	-.4(2)	.9(2)	-.1(1)
C(13)	.0759(4)	.5890(4)	-.1974(4)	4.7(2)	2.6(2)	3.7(2)	.1(2)	.3(2)	.2(2)
C(14)	-.0103(4)	.5175(3)	-.1768(3)	3.5(2)	2.7(2)	3.0(2)	.2(1)	-.1(1)	-.2(1)
C(15)	-.1322(5)	.5598(4)	-.1978(5)	4.1(2)	3.6(2)	6.5(3)	1.0(2)	-.4(2)	.5(2)
C(21)	.0987(5)	.0915(6)	.3983(4)	4.9(3)	9.6(4)	3.1(2)	-.5(3)	1.0(2)	1.0(2)
C(22)	.0566(4)	.1099(4)	.2719(4)	3.4(2)	3.3(2)	3.2(2)	.2(1)	1.0(1)	.4(1)
C(23)	-.0578(4)	.0961(4)	.2191(4)	3.2(2)	3.5(2)	4.0(2)	-.1(1)	1.3(2)	.3(2)
C(24)	-.1082(3)	.1071(3)	.1025(4)	2.5(2)	2.1(1)	4.2(2)	-.1(1)	.7(1)	.0(1)
C(25)	-.2344(4)	.0799(4)	.0624(5)	2.3(2)	5.4(2)	5.7(3)	-.7(2)	.8(2)	.0(2)
C(31)	-.0738(4)	.3431(3)	-.1223(4)	2.6(2)	3.3(2)	3.4(2)	.1(1)	-.0(1)	.3(1)
C(32)	-.0325(3)	.2280(3)	-.1369(4)	2.6(2)	3.1(2)	2.8(2)	-.1(1)	-.0(1)	-.1(1)
C(33)	-.0984(4)	.1426(4)	-.0894(4)	2.8(2)	3.4(2)	3.6(2)	-.7(1)	-.2(1)	-.0(2)
C(41)	.3402(3)	.2119(3)	.0339(4)	2.2(1)	3.4(2)	3.2(2)	-.2(1)	.2(1)	-.2(1)
C(42)	.4581(4)	.1620(4)	.0483(5)	2.8(2)	5.5(2)	5.9(3)	.9(2)	1.2(2)	1.4(2)

ATOM	X	Y	Z	B
H(11)	.044(5)	.657(5)	-.219(5)	5.00000
H(21)	-.114(5)	.085(5)	.270(5)	5.00000
H(31)	-.142(5)	.362(5)	-.179(5)	5.00000
H(32)	-.087(5)	.358(5)	-.043(5)	5.00000
H(33)	-.047(5)	.213(5)	-.215(5)	5.00000
H(34)	-.176(6)	.175(4)	-.095(5)	5.00000
H(35)	-.082(5)	.070(5)	-.128(5)	5.00000

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4(B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}l^2c^{*2} - 2B_{12}hka^{*}b^{*} - 2B_{13}hla^{*}c^{*} - 2B_{23}k\ell b^{*}c^{*})].$$

Table Q. Final Atomic Positional and Thermal Parameters for $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot 2\text{CH}_3\text{CN}$.^a

ATOM	X	Y	Z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Cu(1)	.04051(3)	.03045(6)	.12259(4)	3.96(3)	2.87(2)	2.78(2)	-.18(2)	.81(2)	.20(2)
O1	0.00	.1051(4)	.25	4.3(2)	2.4(2)	3.4(2)	0.00	1.0(1)	0.00
N1	.0690(2)	.2017(4)	.0934(3)	4.2(2)	3.5(2)	3.6(2)	.0(1)	1.0(1)	.3(1)
O2	.0817(2)	-.0329(3)	-.0097(3)	4.3(2)	3.9(2)	4.2(1)	-.3(1)	1.5(1)	-.4(1)
O3	.0253(2)	-.1430(3)	.1669(3)	4.9(2)	3.4(1)	3.7(1)	-.1(1)	1.2(1)	.0(1)
C1	0.00	.2319(9)	.25	14.2(9)	2.8(4)	12.1(8)	0.00	10.7(8)	0.00
C2	.0372(4)	.2955(5)	.1661(5)	7.6(3)	2.6(2)	4.9(2)	.1(2)	2.8(2)	.0(2)
C3	.1129(3)	.2365(5)	.0225(4)	4.1(2)	3.7(2)	4.1(2)	-.2(2)	.8(2)	.2(2)
C4	.1454(2)	.1557(5)	-.0538(4)	3.5(2)	4.2(2)	3.6(2)	.2(2)	.9(2)	.3(2)
C5	.1967(3)	.2087(6)	-.1194(6)	5.1(3)	4.7(3)	6.2(3)	-.5(2)	2.3(2)	.2(3)
C6	.2301(3)	.1388(8)	-.1970(5)	4.6(3)	6.9(4)	5.9(3)	-.1(3)	2.8(2)	.8(3)
C7	.2125(3)	.0135(7)	-.2114(5)	4.0(2)	7.2(4)	5.2(3)	1.0(2)	2.3(2)	-.1(2)
C8	.1629(3)	-.0429(6)	-.1494(5)	4.3(2)	4.9(3)	4.7(2)	.5(2)	1.5(2)	-.4(2)
C9	.1283(2)	.0272(6)	-.0673(4)	3.4(2)	4.5(2)	2.8(2)	.3(2)	.8(1)	-.0(2)
C10	0.00	-.1967(7)	.25	4.4(3)	3.2(3)	4.1(3)	0.00	.4(3)	0.00
C11	0.00	-.3393(8)	.25	8.9(6)	2.6(3)	7.0(5)	0.00	2.6(4)	0.00
NSOLV	.1461(5)	.4552(8)	.3972(8)	11.3(5)	6.8(4)	9.2(5)	-.8(4)	1.7(4)	-.6(4)
C1SLV	.1513(4)	.3910(7)	.4754(7)	6.7(4)	5.3(4)	7.5(4)	-1.9(3)	1.6(3)	-1.2(3)
C2SLV	.1575(5)	.306(1)	.5710(8)	9.2(5)	9.8(6)	8.1(5)	-3.6(4)	.8(4)	1.6(4)

ATOM	X	Y	Z	B
H2	.079(3)	.330(6)	.222(5)	5.00
H3	.044(3)	.373(7)	.139(5)	5.00
H4	.127(3)	.319(6)	.019(5)	5.00
H5	.203(3)	.279(6)	-.114(5)	5.00
H6	.266(3)	.170(6)	-.236(5)	5.00
H7	.237(3)	-.042(6)	-.259(6)	5.00
H8	.155(3)	-.137(7)	-.160(5)	5.00

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4(B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}l^2c^{*2} - 2B_{12}hka^{*}b^{*} - 2B_{13}hla^{*}c^{*} - 2B_{23}k\ell b^{*}c^{*})].$$

Table R. Final Atomic Positional and Thermal Parameters for $\text{Cu}_2(\text{Dapsa})(\text{OAc}) \cdot \text{CH}_3\text{OH}$.^a

ATOM	X	Y	Z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Cu(1)	.11909(7)	.07110(4)	-.03624(3)	2.37(3)	4.10(3)	4.82(4)	-.04(3)	-.25(3)	.20(3)
Cu(2)	.13136(7)	.20044(4)	.07754(3)	2.56(3)	3.79(3)	5.32(4)	.35(3)	-.18(3)	.06(3)
O(1)	.0502(4)	.1448(2)	.0151(2)	2.6(2)	4.6(2)	5.3(2)	.9(1)	-1.8(1)	-.1(2)
O(2)	.1856(4)	.0074(2)	-.0956(2)	2.9(2)	5.9(2)	6.1(3)	.1(2)	-.1(2)	-1.0(2)
O(2')	.2127(4)	.2625(2)	.1350(2)	3.6(2)	3.9(2)	6.2(3)	.4(2)	-.7(2)	-.5(2)
O(3)	.3021(4)	.0718(2)	-.0018(2)	2.8(2)	5.5(2)	6.4(3)	.7(2)	-.3(2)	-1.5(2)
O(3')	.3067(4)	.1512(2)	.0725(2)	2.7(2)	5.4(2)	6.2(3)	.6(2)	-.8(2)	-1.4(2)
OSOLV	.014(1)	.2257(6)	.3489(6)	11.8(6)	12.1(7)	24.6(9)	2.1(5)	9.6(7)	2.8(7)
N(1)	-.0683(5)	.0617(3)	-.0629(2)	3.2(2)	3.8(2)	4.9(3)	.3(2)	-.2(2)	.6(2)
N(1')	-.0411(5)	.2513(3)	.0782(2)	3.7(2)	4.0(2)	4.6(3)	.2(2)	-.5(2)	.7(2)
CSOLV	.078(1)	.2819(8)	.3324(5)	5.4(4)	11.0(7)	12.3(8)	-1.4(5)	.1(5)	1.5(7)

ATOM	X	Y	Z	B
C(1)	-.0780(7)	.1729(4)	-.0045(3)	4.7(1)
C(2)	-.1625(6)	.1104(4)	-.0284(3)	4.3(1)
C(2')	-.1475(6)	.2139(3)	.0439(3)	4.3(1)
C(3)	-.1131(7)	.0190(3)	-.1020(3)	4.2(1)
C(3')	-.0646(7)	.3129(4)	.1038(3)	4.5(1)
C(4)	-.0312(6)	-.0306(3)	-.1361(3)	3.9(1)
C(4')	.0282(6)	.3493(3)	.1425(3)	4.1(1)
C(5)	-.0962(7)	-.0782(4)	-.1764(3)	5.1(2)
C(5')	-.0161(8)	.4167(4)	.1677(3)	5.4(2)
C(6)	-.0272(7)	-.1271(4)	-.2092(3)	5.0(1)
C(6')	.0600(8)	.4542(4)	.2076(3)	5.7(2)
C(7)	.1144(7)	-.1283(3)	-.2066(3)	4.9(1)
C(7')	.1858(8)	.4246(4)	.2258(4)	5.8(2)
C(8)	.1833(7)	-.0832(4)	-.1688(3)	4.8(1)
C(8')	.2320(7)	.3596(4)	.2012(3)	5.2(1)
C(9)	.1146(6)	-.0330(3)	-.1322(3)	4.0(1)
C(9')	.1574(6)	.3217(3)	.1589(3)	4.1(1)
C(10)	.3568(6)	.1041(3)	.0398(3)	3.7(1)
C(11)	.5044(8)	.0824(4)	.0541(4)	6.5(2)

Table R. (Continued).

ATOM	X	Y	Z	B
HC1	-.06070	.20610	-.03760	5.00
HC2	-.23310	.12630	-.05430	5.00
HC2	-.20340	.08440	.00330	5.00
HC2'	-.20180	.18110	.06790	5.00
HC2''	-.21300	.25000	.02760	5.00
HC3	-.21140	.02070	-.10950	5.00
HC3'	-.15070	.33710	.09500	5.00
HC5	-.19420	-.07520	-.17940	5.00
HC5'	-.10290	.43570	.15530	5.00
HC6	-.07820	-.16040	-.23520	5.00
HC6'	.02960	.50060	.22400	5.00
HC7	.16980	-.16200	-.23050	5.00
HC7'	.24130	.44880	.25790	5.00
HC8	.28400	-.08370	-.16710	5.00
HC8'	.32390	.34040	.21090	5.00

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4 (B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}\ell^2c^{*2} - 2B_{12}hka^*b^* - 2B_{13}h\ell a^*c^* - 2B_{23}k\ell b^*c^*)].$$

Table S. Final Atomic Positional and Thermal Parameters for $\text{Cu}_2(\text{Dapsa})(\text{OAc})$.^a

ATOM	X	Y	Z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Cu(1)	.22570(5)	.16409(5)	.0909(1)	3.04(5)	3.94(6)	3.60(5)	-.15(4)	.12(4)	-.61(4)
Cu(2)	.03216(5)	.16661(5)	.0857(1)	3.03(5)	3.57(6)	3.96(5)	-.24(4)	.43(4)	-.56(4)
Cu(3)	.48712(5)	-.07680(6)	.3960(1)	2.86(5)	5.12(7)	2.84(5)	-.24(4)	.03(4)	.29(4)
Cu(4)	.29366(5)	-.07764(6)	.4017(1)	2.77(5)	5.78(7)	3.08(5)	-.17(4)	.09(4)	.21(5)
O11	.1113(3)	.1929(3)	.1425(6)	3.6(3)	3.4(3)	5.2(3)	-.7(2)	-.0(2)	-1.4(2)
O21	.3190(3)	.1439(3)	.0293(6)	3.2(3)	5.1(3)	4.7(3)	-.1(2)	.5(2)	-.8(3)
O31	.1849(3)	.0902(3)	-.0066(7)	3.6(3)	4.4(3)	8.1(4)	-1.2(2)	1.2(3)	-2.1(3)
O2'1	-.0653(3)	.1520(3)	.0088(6)	2.9(3)	5.1(3)	5.0(3)	-.2(2)	-.1(2)	-1.4(3)
O3'1	.0624(3)	.0890(3)	.0014(8)	3.9(3)	4.0(3)	8.6(4)	-.1(2)	.0(3)	-3.0(3)
O12	.3952(3)	-.0871(3)	.4751(5)	3.5(3)	7.2(4)	2.5(2)	-.3(3)	-.6(2)	1.1(3)
O22	.5792(3)	-.0748(3)	.3222(6)	2.9(2)	6.1(4)	4.0(3)	-.5(2)	.4(2)	-.0(3)
O32	.4415(3)	-.0561(4)	.2167(6)	3.9(3)	9.8(5)	3.1(3)	.3(3)	-.1(2)	1.3(3)
O2'2	.1930(3)	-.0731(3)	.3320(6)	2.8(3)	8.0(4)	4.5(3)	.1(3)	.0(2)	.6(3)
O3'2	.3146(3)	-.0549(4)	.2228(6)	3.9(3)	10.2(5)	3.4(3)	-.1(3)	-.7(2)	1.2(3)
N11	.2654(4)	.2331(4)	.2024(7)	3.1(3)	4.6(4)	4.4(4)	-.7(3)	.0(3)	-.7(3)
N1'1	.0042(4)	.2367(4)	.1983(7)	4.0(3)	4.5(4)	3.6(3)	-.4(3)	.3(3)	-1.7(3)
N12	.5310(4)	-.0987(4)	.5791(7)	3.1(3)	5.8(4)	3.2(3)	.1(3)	-.5(2)	.3(3)
N1'2	.2716(4)	-.1010(4)	.5793(7)	3.3(3)	6.4(5)	3.4(3)	.1(3)	1.0(3)	.0(3)

ATOM	X	Y	Z	B
C11	.1352(5)	.2559(5)	.1973(9)	4.0(2)
C21	.2103(5)	.2627(5)	.284(1)	4.6(2)
C2'1	.0690(5)	.2648(5)	.283(1)	4.7(2)
C31	.3323(5)	.2575(5)	.2076(9)	4.3(2)
C3'1	-.0611(5)	.2598(5)	.2066(9)	4.4(2)
C41	.3900(5)	.2312(4)	.1341(9)	4.0(2)
C4'1	-.1270(5)	.2331(4)	.1303(9)	4.2(2)
C51	.4597(5)	.2643(5)	.151(1)	4.8(2)
C5'1	-.1966(6)	.2638(5)	.155(1)	5.3(2)
C61	.5184(6)	.2431(6)	.086(1)	5.7(2)
C6'1	-.2620(6)	.2417(5)	.087(1)	5.3(2)
C71	.5101(6)	.1888(5)	.001(1)	5.1(2)
C7'1	-.2603(6)	.1917(5)	-.000(1)	5.2(2)
C81	.4416(5)	.1553(5)	-.0151(9)	4.5(2)
C8'1	-.1953(5)	.1596(5)	-.028(9)	4.3(2)
C91	.3816(5)	.1773(4)	.0499(8)	3.4(2)
C9'1	-.1266(5)	.1817(4)	.0403(9)	3.9(2)

Table S. (Continued).

ATOM	X	Y	Z	B
C12	.4034(6)	-.1092(5)	.607(1)	5.4(2)
C22	.4764(6)	-.0968(5)	.680(1)	5.2(2)
C2'2	.3384(6)	-.1072(5)	.681(1)	5.8(2)
C32	.6008(5)	-.0882(4)	.6211(9)	4.1(2)
C3'2	.2081(5)	-.1090(5)	.6241(9)	4.3(2)
C42	.6589(5)	-.0810(4)	.5294(9)	4.1(2)
C4'2	.1389(5)	-.0994(5)	.540(1)	4.4(2)
C52	.7339(6)	-.0777(5)	.597(1)	5.2(2)
C5'2	.0722(6)	-.1083(5)	.606(1)	5.3(2)
C62	.7923(6)	-.0736(5)	.516(1)	5.8(2)
C6'2	.0037(7)	-.0998(6)	.531(1)	6.6(3)
C72	.7802(6)	-.0716(6)	.376(1)	6.0(2)
C7'2	-.0000(7)	-.0822(6)	.395(1)	6.7(3)
C82	.7041(5)	-.0729(5)	.389(1)	4.5(2)
C8'2	.0626(6)	-.0718(5)	.331(1)	5.8(2)
C92	.6462(5)	-.0762(4)	.3888(8)	3.5(2)
C9'2	.1353(5)	-.0814(4)	.4036(9)	4.2(2)
C101	.1233(5)	.0636(5)	-.0183(9)	4.2(2)
C111	.1198(6)	-.0054(6)	-.071(1)	6.2(2)
C102	.3762(5)	-.0467(4)	.1637(9)	3.8(2)
C112	.3673(6)	-.0208(5)	.022(1)	5.1(2)

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4(B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}l^2c^{*2} - 2B_{12}hka^{*}b^{*} - 2B_{13}hla^{*}c^{*} - 2B_{23}k\ell b^{*}c^{*})].$$

Table T. Final Atomic Positional and Thermal Parameters for Cu(DapsaH)·CH₃CN.^a

ATOM	X	Y	Z	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Cu	-.0097(2)	.1162(1)	.0662(3)	3.62(9)	2.73(7)	2.58(7)	.2(1)	.47(6)	.1(1)

ATOM	X	Y	Z	B
O1	.0802(4)	.1724(6)	-.453(2)	5.4(3)
O11	-.1156(7)	.1152(7)	.240(1)	3.8(2)
O21	.1032(7)	.1045(6)	.235(1)	3.6(2)
N11	-.102(1)	.1688(6)	-.090(2)	3.2(3)
N21	.071(1)	.0728(7)	-.121(2)	3.5(3)
C1	-.012(1)	.1389(7)	-.372(2)	3.3(4)
C11	-.051(1)	.1993(8)	-.245(2)	3.5(4)
C12	-.202(1)	.1423(8)	-.080(2)	3.6(4)
C13	-.260(1)	.1652(8)	.076(2)	3.3(3)
C14	-.374(1)	.1822(9)	.068(2)	4.9(4)
C15	-.436(2)	.166(1)	.211(3)	5.8(5)
C16	-.347(1)	.1356(9)	.398(2)	4.8(4)
C17	-.279(1)	.118(1)	.369(2)	4.2(3)
C18	-.214(1)	.1337(8)	.225(2)	3.6(3)
C21	.009(1)	.0672(9)	-.287(2)	4.3(4)
C22	.168(1)	.0467(8)	-.106(2)	3.8(4)
C23	.226(1)	.0444(8)	.054(2)	3.4(3)
C24	.323(1)	.0068(8)	.042(2)	3.7(4)
C25	.394(1)	.002(1)	.182(3)	5.4(4)
C26	.359(1)	.028(1)	.351(2)	5.0(4)
C27	.262(1)	.0648(9)	.360(2)	3.9(4)
C28	.196(1)	.0728(8)	.210(2)	3.3(3)
NSOLV	.405(2)	.355(1)	.215(3)	9.2(6)
C1SLV	.351(2)	.317(1)	.286(3)	6.7(5)
C2SLV	.275(2)	.269(1)	.378(3)	10.1(7)

^a The form of the thermal ellipsoid expression is:

$$\exp [1/4(B_{11}h^2a^{*2} - B_{22}k^2b^{*2} - B_{33}l^2c^{*2} - 2B_{12}hka^{*}b^{*} - 2B_{13}hla^{*}c^{*} - 2B_{23}klb^{*}c^{*})].$$

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